QUANTUM MECHANICS

for

CSIR-UGC-NET/JRF | GATE

TIFR | JEST | BARC | IISc | JNU | SLET | PhD Entrance

First Edition : Nov 2015

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Preface to the First Edition

Quantum Mechanics form an important part of the syllabus for the graduate and post-graduate physics courses of various Indian Universities. While teaching this subject, particularly in physics honours classes, we very often refer to various standard books for the various topics of Quantum Mechanics. But none of these books is fully sufficient for the preparation of different competitive examinations at national and state levels such as CSIR-UGC-NET/JRF, GATE, TIFR, JEST, BARC etc. In all these competitive examinations, the section of Quantum Mechanics carries a high percentage of weightage of the total marks as follows:

- In every year CSIR-UGC-NET paper contains questions of at least 35 to 40 marks from this section out 200 marks.
- In every year GATE paper contains questions of at least 12 to 15 marks from this section out 100 marks.

The purpose of the present book is to provide a brief discussion of every important topic of the Quantum Mechanics syllabus. Each chapter contains a significant number of solved problems some of which contain subtle points, not explicit in the text and hence will help the students to attain a deeper understanding of the ideas presented in the book. Moreover, the problems that are asked in CSIR-UGC-NET examinations till date, has been solved at the end of each chapter. Besides this, problems that are asked in GATE, TIFR, JEST till date, has been given at the end of each chapter for the practice of the students. This will surely help the student to enhance their self-confidence.

It is hoped that the book will be able to meet up all the requirements of the students preparing for the various competitive examinations. However, any constructive criticism and suggestions for the improvement of the book will always be highly appreciated. Much care has been taken to minimize the typographical errors, yet if any noticed, then your suggestions are invited with a view to improve the book in future editions.

The author (Surajit Paul) would like to thank my parents, family members, students, friends and specially Anwesha Chakraborty who have given constant support in the development of the book. Thanks are due to the unit of *Career Endeavour Publications* for making sincere efforts towards timely publication of the book. Thanks to Mr. Surajit Kuila for his constructive support in doing corrections and proofreading. Last but not the list, a very special thanks to Mohammad Firoz for typing, formatting and designing of the book.

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Chapter 1

Origin of Quantum Mechanics

1.1 Introduction :

At the end of the 19th century, physics consisted essentially of Newton's Classical mechanics and Maxwell's theory of electromagnetism. Classical mechanics was used to predict the dynamics of material bodies and Maxwell's electromagnetism provided the proper frame work to study radiation. In fact, matter and radiation were described in terms of particles and waves and the interactions between matter and radiation were well explained by Lorentz force and Thermodynamics. The overhelming success of classical physics, classical electromagnetism made us believe that the ultimate description of nature has been acheived and every physical phenomena can be explained in the general framework of radition and matter.

In the 20th century, classical physics has been challenged by two major fronts:

(1) **Relativistic domain:** Einstein's theory of relativity showed that the validity of Newtonian mechanics ceases at a speed that is comparable to light.

(2) **Microscopic domain:** Classical physics fails in providing the proper explaination for several newly discovered phenomena microscopic domain such as black body radiation, photoelectric effect, atomic stability, atomic spectroscopy and new concepts has to be invoked to describe these phenomenas.

In 1900, Max planck introduced the concept of the quantum of energy to explain the phenomena of Black body radiation and postulated that the energy exchange between the radiation and its surroundings takes place in discrete or quantized amounts. He argued that the energy exchange between the e.m. wave of frequanecy ν and matter occurs only in integer multiple of $h\nu$ which is called the quanta of energy.

In 1905, Einstein recognized that the idea of quantization of light is valid also for light and postulated that light is made of discrete bits of energy (or tiny particles), called photons, each of energy $h\nu$ and successfully explained the photoelectric effect. A series of breakthroughs due to Planck, Einstein, Bohr, Compton gave both the theoretical background as well as experimental confirmation of the particle aspects of waves at the microscopic level. In 1923, De-broglie postulated that not only does the radiation exhibits particle like behaviour but conversely material particles show the wave like behaviour. This concept was experimentally confirmed by Davisson and Germer in 1927.

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Generally there are two independent formulations of quantum mechanics. The first formulation called matrix mechanics, was devoloped by Heisenberg in 1925 and second formulation called wave mechanics, was devoloped by Schrodinger in 1926, which is the generalization of De-broglie postulate. These two different formulations of quantum mechanics were shown to be equivalent. Moreover, Dirac has suggested a more general formulation of quantum mechanics which deals with abstract objects like kets (state vectors), bras and operators. The representation of Dirac formalism in a continuous basis i.e. in the position and momentum representation gives back the Schrodinger's wave mechanics and the representation of Dirac formalism in a discrete basis gives the Heisenberg's matrix formulation.

1.2 Particle aspect of radiation :

According to classical physics, a particle is characterized by an energy E and a momentum $\vec{p}$,whereas a wave is characterized by an amplitude and wave vector $\vec{k}$ that specifies the direction of the propagation of wave. For instance, the particle and wave properties are mutually exclusive and wave can exchange any amount of energy with particles. Now, we will see that how the phenomenas like photoelectric effect, compton effect shows the particle aspect of radiation.

Photoelctric Effect:

During his experiments on e.m. waves in 1887, Hertz noticed that sparks occurred more rapidly in the air gap of the transmitter when an ultraviolet light is directed at one of the metal balls used in that experiment. Phillip Lenard, a student of Hertz studied the phenomena. He soon discovered that when the frequency of light is sufficiently high, electrons are emitted from the metal surface.

The phenomena in which electrons are emitted from the metal surface (e.g. Na, K, Cs etc.) when irradiated with light (photon) is called "Photo-electric effect". The metals which exhibits this phenomena are called "Photo-sensitive materials" and the emitted electrons are called "Photo-electrons". The existence of photo electric effect is not surprising. Light waves carry energy and some of the energy absorbed by the metal gets concentrated on a particular electron and reappear as their kinetic energy.

Lenard's Experiment :

Lenard's experimental arrangement is as shown in figure above. Two plane metal plates C and D are mounted in an evacuated tube. Plate G is coated with photosensitive metal and maintained at a negative whereas A another metal plate and kept at zero potential. The beam of negative ions emitted from C can pass through a hole in A. UV-radiation is incident on C through the quartz window W fitted to the side tube G and negative ions are emitted. These are attracted to A and a part of it passing through the hole in A is collated at D. The resulting electric current can be detected by an electrometer E.

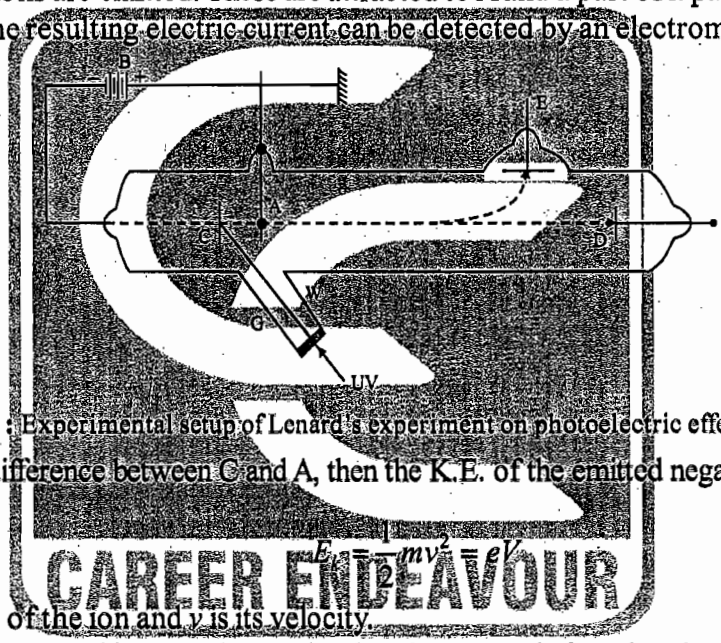

Figure : Experimental setup of Lenard's experiment on photoelectric effect

If V be the potential difference between C and A, then the K.E. of the emitted negative ions is,

$$E_k = \frac{1}{2}mv^2 = eV$$

where, m is the mass of the ion and v is its velocity.

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Further, if a positive potential is applied to C, the electric current is found to decrease with the increase of positive potential. Ultimately a stage comes when in a particular p.d. (V_s) the current becomes zero. Then, this V_s is called stopping potential. Electrons of all velocities up to the maximum v_m are stopped from reaching A. Then

$$E_{k,\max} = \frac{1}{2}mv_{\max}^2 = eV_s$$

Some experimental observations:

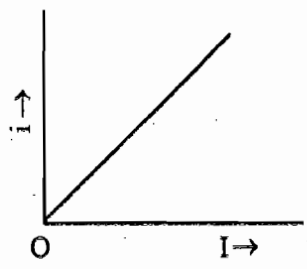

Figure : Variation of photo current (i) with the intensity of radiation (I)

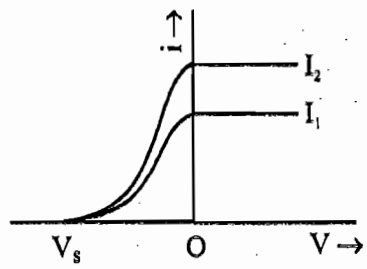

Figure : Variation of photo current (i) with Potential difference (V)

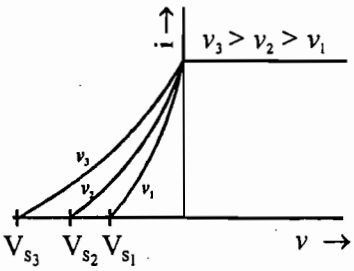

Figure : Plot of photocurrent (i) against Potential difference V showing the variation of stopping potential (V_s) with frequency (ν) of radiation.

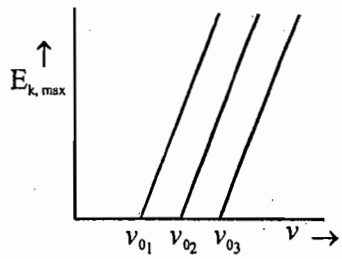

Figure : Plot of $E_{k,max}$ against ν.

(i) There is a certain minimum frequency ν_0 of incident radiation below which there is no emission of photo-electrons regardless of the intensity of the incident radiation. This frequency is known as threshold frequency which depends on the material and the nature of the emitting surface.

(ii) The maximum velocity or kinetic energy of the emitted photoelectrons depends on the frequency of the incident light, not on it's intensity i.e. blue light results in faster electrons than red light. The kinetic energy of the ejected electron increases linearly with incident frequency.

(iii) The emission of photo-electrons is instantaneous i.e. no time interval between arrival of light at the metal surface and emission of photo-electrons, no matter how feeble the incident light is.

(iv) At a fixed frequency, the number of ejected electrons increases with the intensity of the light but does not depend on its frequency.

Failures of Classical E.M. theory:

(i) According to wave theory, photo-electric emission should occur for any frequency of light, no concept of threshold frequency.

(ii) According to wave theory, the energy of the incident light is distributed over the entire wave front. So, electrons will take some time to eject from the surface i.e. no concept of instantaneous emission.

(iii) The electric field and magnetic field of the incident light wave exert forces to liberate electrons from the metal surface. So, the light of higher intensity consists of stronger fields and should give higher velocity to the photoelectrons.

Einstein's hypothesis:

(i) The emission and absorption of radiation takes place in descrete quanta of energy $\varepsilon = h\nu$.

(ii) Energy in light is not spread out over the entire wavefront but is concentrated in small packets known as 'photons'. The incident photon on the metal surface can transfer the whole energy to one electron without any time lag.

(iii) A certain minimum energy called the work function W_0 is required to release an electron from the metal surface.

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Photo-electric equation:

When a radiation of frequency ν is incident on the metal surface in vaccum, it can be either be reflected from the metal surface or it can be completely absorbed by an electron. In the second case, the electron can be knocked out of the surface. The emission of electron from the metal surface is possible only if $h\nu > W_0$. The remaining energy $(h\nu - W_0)$ can be utilized to impart kinetic energy of the emitted electrons.

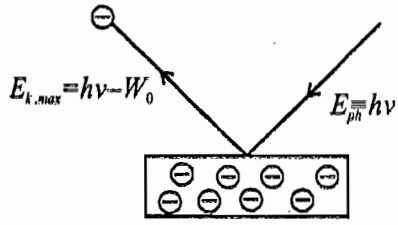

Figure : Mechanism of Photoelectric effect.

So, the maximum kinetic energy of the emitted electrons is

$$E_{k,\max} = \frac{1}{2}mv_{\max}^2 = h\nu - W_0 = h\nu - h\nu_0$$

where 'm' is the rest mass of the electron, $v_{\max}$ is the maximum velocity of the emitted electrons and ν_0 is the threshold frequency. This is the well-known Einstein's photo-electric equation.

Explaination of Photoelectric effect:

(i) If $\nu < \nu_0$, the maximum kinetic energy of the emitted photo-elctron is negative. This means that no electrons could be emiited if the frequency of the incident photon ν is less than the threshold frequency ν_0.

(ii) Above the threshold frequency, the maximum kinetic energy of the emitted photoelectrons varies linearly with ν, it does not depend on the intensity of the incident radiation.

(iii) An increase in the frequency of the incident radiation for a fixed frequency ν, is equivalent to the increase in the number of photon and not energy.

(iv) Above the threshold frequency, the incident photon is absorbed at an instant by the electron and is emitted instantaneously.

Example 1. Calculate the number of photons emitted per second by a 100-watt sodium lamp. [Assume $\lambda = 5893\,\text{Å}$ of sodium light]

Soln. Energy of a photon,

$$\in = h\nu = \frac{hc}{\lambda} = \frac{1240\,eV - nm}{589.3\,nm} = 2.1\,eV = 3.37\times10^{-19}\,J$$

Now, the rate of energy emission from a 100-watt lamp is 100 J/s

Number of photons emitted per second is $\frac{100}{3.37\times10^{-19}} = 2.96\times10^{20}$

Example 2. The kinetic energies of photoelectrons range from zero to $4.0\times10^{-19}\,J$ when light of wavelength 3000Å falls on a metal surface. What is the stopping potential? What is the threshold wavelength?

Soln. Maximum kinetic energy of photoelectrons is

$$E_{k,\max} = \frac{4.0\times10^{-19}}{1.6\times10^{-19}}eV = 2.5\,eV$$

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If V_s be the stopping potential, then

$$eV_s = E_{k,\max} \Rightarrow V_s = \frac{2.5\,eV}{e} = 2.5V$$

Again, $eV_s = h\nu - h\nu_0 = \frac{hc}{\lambda} - \frac{hc}{\lambda_0} \Rightarrow 2.5\,eV = \frac{12.4\times10^3\,eV\text{Å}}{3000\,\text{Å}} - \frac{12.4\times10^3\,eV\text{Å}}{\lambda_0} \Rightarrow \lambda_0 = 7590\,\text{Å}$

Example 3. The threshold wavelength for photoelectric emission in tungsten is 230 nm. What wavelength of incident light must be used in order to eject electrons with a maximum velocity of $5\times10^5\ m/s$. [Mass of the electron= $9.1\times10^{-31}\,kg$]

Soln. From the photoelectric equation,

$$h\nu = \left(\frac{1}{2}mv^2\right)_{\max} + h\nu_0 \Rightarrow h\frac{c}{\lambda} = \left(\frac{1}{2}mv^2\right)_{\max} + h\frac{c}{\lambda_0}$$

$$\Rightarrow \frac{19.88\times10^{-26}}{\lambda}=\frac{19.88\times10^{-26}}{230\times10^{-9}}+113.75\times10^{-21} \Rightarrow \lambda=0.0203\times10^{-5}\,m$$

Therefore, the required wavelength = 2030Å.

Example 4. The work function of aluminium is 4.2 eV. Calculate the kinetic energy of the fastest and slowest photoelectrons, the stopping potential and the cut-off wavelength when light of wavelength 2000Å falls on a clean aluminium surface.

Soln. According to Einstein's photoelectric equation, the KE of the fastest electron is given by

$$E_{k,\max}=h\nu-W_0=(6.2-4.2)\text{ eV}=2\text{ eV}$$

The kinetic energy of the slowest photoelectrons is zero.

Now, the stopping potential is equal to the maximum KE of the photoelectrons, i.e. 2.0 eV.

Now, cut-off frequency, $\nu_0=\frac{w_0}{h}=\frac{4.2\times1.6\times10^{-19}}{6.63\times10^{-34}}J=1.0\times10^{15}/s$

cut-off wavelength, $\lambda_0=\frac{c}{\nu_0}=\frac{3.0\times10^8}{1.0\times10^{15}}=3.0\times10^{-7}\,m=3000\,\text{Å}$

Example 5. What is the maximum kinetic energy of photoelectrons released from the surface of lithium by electromagnetic radiation whose electric field E is given by

$$E=A(1+\sin\omega t)\cos\omega_0 t$$

where, A is a constant, $\omega=6\times10^{14}/s$, $\omega_0=3.6\times10^{15}/s$, the work function of lithium is 2.4 eV

Soln. Here, $E=A\cos\omega_0 t+A\sin\omega t\cos\omega_0 t$

$$=A\cos\omega_0 t+\frac{A}{2}\left\{\sin(\omega+\omega_0)t-\sin(\omega_0-\omega)t\right\}$$

The kinetic energy of the emitted photo electrons is directly proportional to the frequency of the incident light.

Therefore, the maximum kinetic energy will correspond to $(\omega_0+\omega)$

The maximum KE $=\hbar(\omega_0+\omega)-W_0=0.38\,eV$

Example 6. Ultraviolet light of wavelength 350 nm and intensity 1.00 W/m² is directed at a potassium surface. If 0.50% of the incident photons produce photoelectrons, how many photoelectrons are emitted per second if the potassium surface has an area of 1.00 cm².

Soln. Energy of the single photon is

$$E_p=\frac{1240\,eV-nm}{350nm}=3.5\,eV=5.68\times10^{-19}J$$

Therefore, the number of photons that reach the surface per second is,

$$n_p=\frac{\text{Power}}{E_p}=\frac{\text{Intensity}\times\text{Area}}{E_p}=\frac{\left(1.00\,W/m^2\right)\times\left(1.00\times10^{-4}\,m^2\right)}{5.68\times10^{-19}J}$$

Therefore, the rate of emission of photoelectrons is,

$$n_e=(0.0050)n_p=8.8\times10^{11}\text{ photoelectron/s}$$

Example 7. Calculate the magnitude of the linear momentum of a photon of radiation having electric field described by $\vec{E}=E_0\hat{i}\cos\left[k_0(y+z)-\omega t\right]$.

Soln. The equation for the electric field of an electromagnetic wave can be written as

$$\vec{E}=\vec{E}_0\cos\left(\vec{k}.\vec{r}-\omega t\right)$$

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Thus, $\vec{k} = k_0\hat{j} + k_0\hat{k}$ and $\vec{r} = x\hat{i} + y\hat{j} + z\hat{k}$

The linear momentum of the photon is

$$\vec{p} = \hbar\vec{k} = \hbar\left(k_0\hat{j} + k_0\hat{k}\right)$$

The magnitude of the linear momentum is

$$|\vec{p}| = \hbar\left|k_0\hat{j} + k_0\hat{k}\right| = \sqrt{2}\,\hbar k_0$$

Example 8. Calculate the magnitude of the linear momentum of a photon in a beam of He-Ne laser $(\lambda = 634\ nm)$ in the units of $\frac{eV}{c}$.

Soln. $p = \frac{h}{\lambda} = \frac{hc}{\lambda c} = \frac{1240\ eV\ nm}{(634nm)c} = 1.96\ eV/c$

Example 9. A beam of light of wavelength 420 nm has the same intensity as another beam of light of wavelength 630 nm. The first beam, falling perpendicularly on a certain area of a wall, deposits 12×10^{16} photons per second per square centimeter of the wall. How many photons will the second beam deposit per second per square centimetre of a wall on which it falls perpendicularly.

Soln. The intensity of a wave is defined as the total energy falling per unit area per unit time on a perpendicular cross-section. Thus both the beams will deposit same amount of energy on the one square centimeter area of the wall in one second. If n_1 is the number of photons deposited by the first beam the corresponding energy deposited is

$$E = n_1\left(\frac{hc}{\lambda_1}\right)$$

Similarly, if n_2 is the number of photons deposited by the second beam,

$$E = n_2\left(\frac{hc}{\lambda_2}\right)$$

Thus, $\frac{n_1}{\lambda_1} = \frac{n_2}{\lambda_2} \Rightarrow \frac{12\times10^{16}}{420} = \frac{n_2}{630} \Rightarrow n_2 = \frac{630}{420}\times12\times10^{16} = 18\times10^{16}$

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Example 10. Beam of 450 nm light is incident on a metal having work function 2.0 eV placed in a magnetic field B. The most energetic electrons, emitted perpendicular to the field, are bent in circular arc of radius of 20 cm. Find the value of B.

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Soln. Kinetic energy of the most energetic electrons is

$$E_{k,\max} = \frac{hc}{\lambda} - W_0 = \frac{1240\ eV - nm}{450\ nm} - 2.0\ eV = 0.76\ eV = 1.2\times10^{-19}\ J$$

Linear momentum of the most energetic electrons = $mv = \sqrt{2mK} = 4.67\times10^{-25}\ kg\ m/s$

When a charged particle is sent perpendicular to a magnetic field, it goes along a circle of radius

$$r = \frac{mv}{qB} \Rightarrow B = \frac{mv}{qr} \Rightarrow B = \frac{4.67\times10^{-25}\,kg\ m/s}{\left(1.6\times10^{-19}C\right)\times(0.20m)} = 1.46\times10^{-5}T$$

Compton Effect:

When a beam of monochromatic X-rays of wavelength λ is scattered by a light element (e.g. carbon), it is observed that scattered X-rays have maximum intensities at two wavelengths λ and λ' $(\lambda' > \lambda)$. The radiation at wavelength λ is called unmodified radiation whereas radiation λ' at wavelength is called modified radiation. This phenomenon is known as Compton Effect and the wavelength difference $\lambda' - \lambda$ is called Compton shift. This shift is independent of wavelength λ of the incident beam and the nature of the scatterer but depends on the angle of scattering.

Experiment:

A beam of monochromatic X-rays is allowed to fall on a block of graphite and the intensities of the scattered X-rays are measured as a function of wavelength of X-rays, at different scattering angles.

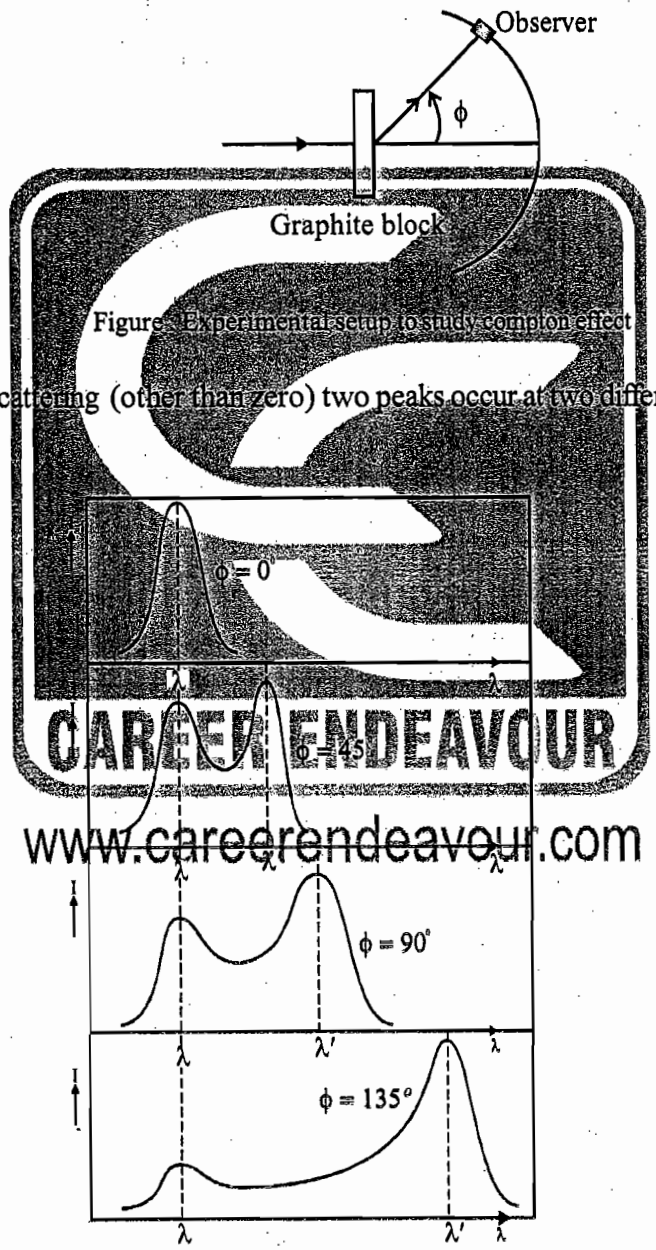

Figure: Experimental setup to study compton effect

For each angle of scattering (other than zero) two peaks occur at two different wavelengths.

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Figure : Variation of intensities of scattered light as a function of wavelength for various scattering angles (ϕ).

Failure of classical theory:

In classical wave theory, X –rays are e.m. waves. If ν is the frequency of the incident X-rays on the material, then they cause electrons in the material to oscillate at the same frequency ν. Hence, the scattered X-radiation should consist of single frequency ν (or single wavelength λ). gain, electrons should radiate X-rays uniformly in all directions and hence, wavelength of the scattered radiation should not vary with scattering angle.

Assumptions:

Compton applied Einstein's quantum theory of light with that assumption that the incident photons posses momentum in addition to energy.

1. The beam of incident monochromatic X-rays of frequency ν consists of streams of photons each of energy $\varepsilon = h\nu$ and momentum $p = \frac{h\nu}{c}$, travelling along the direction of the beam with velocity 'c'.
2. The scattering is due to the elastic collision between photon and the free electron at rest. Hence, the conservation laws of energy and momentum hold good in the scattering process.

Explanation:

We consider a beam of monochromatic X-rays of frequency ν and wavelength λ be incident on a target electron. Let, the incident photon after suffering elastic collision with the free electron, is scattered through an angle ϕ and the electron recoils in a direction θ with the direction of incidence.

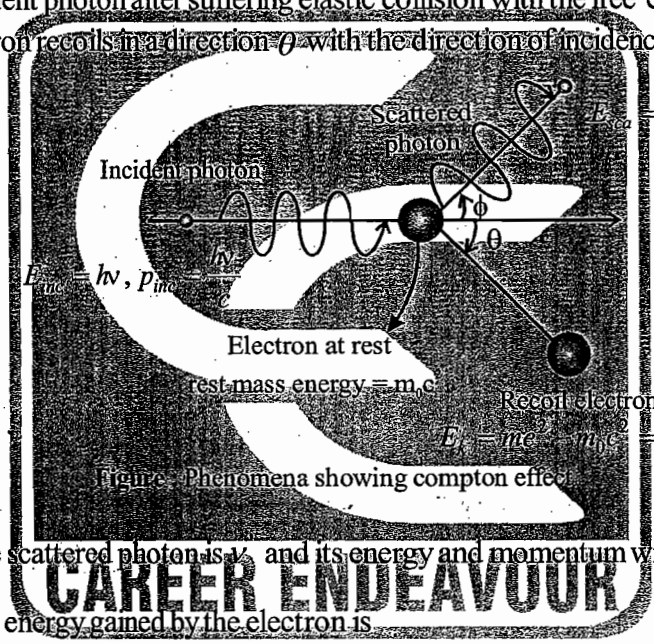

Figure : Phenomena showing compton effect

If the frequency of the scattered photon is ν' and its energy and momentum will be $h\nu'$ and $\frac{h\nu'}{c}$ respectively.

Therefore, the kinetic energy gained by the electron is

$$E_k = mc^2 - m_0c^2 = \frac{m_0c^2}{\sqrt{1-(v/c)^2}} - m_0c^2 \qquad \ldots (2)$$

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Applying law of conservation of energy: $h\nu = h\nu' + E_k$

Applying law of conservation of linear momentum along and perpendicular to the direction of incidence:

$$\frac{h\nu}{c} = \frac{h\nu'}{c}\cos\phi + \frac{m_0v}{\sqrt{1-(v/c)^2}}\cos\theta$$

$$0 = \frac{h\nu'}{c}\sin\phi - \frac{m_0v}{\sqrt{1-(v/c)^2}}\sin\theta \qquad \ldots (3)$$

From the equation (3) we can obtain the compton shift to be,

$$\lambda' - \lambda = \Delta\lambda = \frac{h}{m_0c}(1-\cos\phi) = \lambda_c(1-\cos\phi) \qquad \ldots (4)$$

where, $\lambda_c = 0.02426\,A^0$ is Compton wavelength

Conclusions:

(i) Compton shift is independent of the wavelength of incident radiation and of the nature of the scattering material.

(ii) Compton shift depends on the scattering angle ϕ.

(iii) Larger as the rest mass of the scatterer is smaller.

Relation between ν and ν': $\frac{\nu}{\nu'} = 1 + \frac{h\nu}{m_0 c^2}(1-\cos\phi) = 1 + \alpha(1-\cos\phi)$

Relation between θ and ϕ: $\cot\theta = (1+\alpha)\tan\frac{\phi}{2}$

Kinetic energy of the recoil electron:

$$E_k = h\nu - h\nu' = h\nu\frac{\alpha(1-\cos\phi)}{1+\alpha(1-\cos\phi)} = h\nu\frac{2\alpha\cos^2\theta}{(1+\alpha)^2-\alpha^2\cos^2\theta}$$

Limitations:

(i) Compton effect does not interpret anything about unmodified wavelength. .

(ii) It has been observed that intensities of modified x-rays are greater than the intensities of unmodified X-rays for the lighter elements. But it is reverse for heavier elements. Compton theory does not interpet anything about it.

Example 11. Show that the maximum recoil energy of a free electron of rest mass m0 when struck by a photon of wavelength λ is given by

$$E_{max} = \frac{2m_0c^2\lambda_c^2}{\lambda^2 + 2\lambda_c\lambda}$$

where, λ_c is the Compton wavelength of the electron.

Soln. The recoil electron in the Compton scattering has kinetic energy

$$E = h(\nu - \nu') = hc\left(\frac{1}{\lambda'} - \frac{1}{\lambda}\right)$$

It appears that E will be E_{max} when λ' is the maximum.

$$\therefore \quad E_{max} = hc\left[\frac{1}{\lambda} - \frac{1}{\lambda_{max}}\right] = hc\left[\frac{1}{\lambda} - \frac{1}{\lambda+2\lambda_c}\right] = hc\left[\frac{2\lambda_c}{\lambda^2+2\lambda\lambda_c}\right] = \frac{\left(2m_0c^2\lambda_c^2\right)}{\left(\lambda^2+2\lambda\cdot\lambda_c\right)}$$

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Example 12. A beam of γ-radiation having photon of energy 510 keV is incident on a foil of aluminium. Calculate the wavelenth of radiation at 90° and also the energy and direction of the emission of the corresponding electron.

Soln. Energy of a photon of frequency ν is $\in = h\nu = \frac{hc}{\lambda}$.

Here, $\in = 510\ keV = 510\times10^3\times1.6\times10^{-19}\ J$

$$\therefore \quad \lambda = \frac{hc}{\in} = \frac{6.6\times10^{34}\times3\times10^8}{510\times10^3\times1.6\times10^{-19}} = 2.426\times10^{-12}\ m$$

The wavelength of the scattered radiation is,

$$\lambda' = \lambda + \frac{h}{m_0 c}(1-\cos\phi) = \frac{2.426\times10^{-12} + 6.6\times10^{-34}(1-\cos 90^\circ)}{9.1\times10^{-31}\times3\times3\times10^{8}}$$

$$= 2.426\times10^{-12} + 2.417\times10^{-12} = 4.843\times10^{-12}\,m$$

The energy of the recoil electron is,

$$E = h\nu - h\nu' = h(h-\nu') = \frac{hc(\lambda'-\lambda)}{\lambda\lambda'}$$

$$= \frac{6.60\times10^{-34}\times3\times10^{8}\times\left(4.843\times10^{-12} - 2.426\times10^{-12}\right)}{2.426\times10^{-12}\times4.843\times10^{-12}} = 4.072\times10^{-14}\,J$$

The direction of the recoil electrons is given by,

$$\tan\phi = \frac{\cot\phi/2}{\left(1+\frac{h}{\lambda_{m_0}c}\right)} = \frac{\cot 45^\circ}{1+\frac{6.6\times10^{-34}}{\left(2.426\times10^{-6}\right)\times9.1\times10^{-31}\times\left(3\times10^{8}\right)}} = \frac{1}{1+0.9985} = \frac{1}{1.9985} = 0.5008$$

$$\therefore \quad \phi = \tan^{-1}0.5008 = 26^0 36'$$

Example 13. Show that a free electron at rest cannot absorb a photon.

Soln. If p_{ph} and p_{el} be the momentum of a photon and that of a free electron, then

$$p_{ph} = p_{el} \Rightarrow \frac{h\nu}{c} = P_{el}$$

If E_{ph} and E_{el} be the energies of a photon and a free electron, then

$$E_{ph} = E_{el} \Rightarrow h\nu = \sqrt{(P_{el}c)^2 + (m_0c^2)^2}$$

Thus, the conservation law of momentum breaks down. Hence the result.

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Example 14. A photon of energy $\in$ is scattered from a free electron of mass m_0 and observed at scattering angles greater than $\frac{\pi}{3}$. Show that the energy $\in'$ of the scattered photon is less than $2m_0c^2$, however large the value of $\in$ may be.

Soln. The energy of the scattered photon is,

$$\in' = \frac{\in}{1+2\alpha\sin^2\frac{\phi}{2}} = \frac{\in}{1+\frac{2\in}{m_0c^2}\sin^2\frac{\phi}{2}}$$

For scattering angle $\phi > \frac{\pi}{3}, \sin^2\frac{\phi}{2} > \frac{1}{4}$ as $\sin\phi$ is an increasing function of ϕ. For any value of $\phi > \frac{\phi}{3}, \sin^2\phi > \frac{1}{4} = \frac{k}{4}$ where $k \geq 1$ according as $\phi \geq \frac{\pi}{3}$.

Therefore, the energy of the scattered photon is,

$$\epsilon' = \frac{\epsilon}{1+\frac{2\epsilon}{m_0c^2}\cdot\frac{k}{4}} = \frac{\epsilon}{1+\frac{k\epsilon}{2m_0c^2}} = \frac{2m_0c^2}{\frac{2m_0c^2}{E}+k}$$

Since, $\frac{2m_0c^2}{E}$ is a positive quantity and $k \geq 1$, $\frac{2m_0c^2}{E}+k$ is always greater than 1 and ϵ' is always less than $2m_0c^2$, however large the value of ϵ may be.

1.3. Wave Nature of Matter:

According to classical mechanics, the particle can behave as a particle and wave can behave like a wave. Particle is characterized by energy and momentum and wave is characterized byamplitude and wave vector. In 1923, De-broglie postulated that a moving particle can behave as a wave. The de-broglie wavelength associated with a particle of rest mass 'm_0' moving with a velocity 'v' is given by

$$\lambda = \frac{\hbar}{p} = \frac{\hbar}{\gamma m_0 v}, \quad \text{where } \gamma = \frac{1}{\sqrt{1-\frac{v^2}{c^2}}} \text{ is Lorentz factor}$$

This hypothesis is experimentally verified by Davission-Germer experiment in 1927. If the De-broglie wavelength is comparable to size of the particle, then the wave nature of the particle can be experimentally detected. Otherwise, if the De-broglie wavelength is very small, the wave nature cannot be detected experimentally.

Schrodinger modified the concept wave nature of matter i.e. particle is not like a single plane wave but is like a group of waves i.e. Wave packet. It is just the superposition of waves different wavelengths and frequencies.

Phase Velocity:

A plane wave travelling along positive direction of x-axis can be represented as,

$$\psi(x,t) = A\sin(\omega t - kx) = A\sin\omega\left(t - \frac{x}{v}\right)$$

where, ω is the angular frequency, v is the velocity and A is the amplitude of the wave.

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The phase ϕ of the wave at any time 't' at a distance 'x' from the origin is $\phi(x,t) = (\omega t - kx)$. Phase velocity v_p of the wave is the velocity with which displacement of a given phase, moves in the forward direction. It is also the velocity of a monochromatic wave with which crest or trough of the wave travels in a medium. In a dispersive medium, v_p is different for different wavelengths. The phase velocity of the propagating monochromatic wave is given by, $v_p = \frac{\omega}{k} = \frac{E}{p}$.

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From the relativistic mass energy relation, $v_p = \frac{E}{p} = \frac{\gamma m_0 c^2}{\gamma m_0 v} = \frac{c^2}{v}$

Since, the phase velocity of a de-broglie wave is always greater than the velocity of light in free space. But according to the special theory of relaticvity, no energy can be transmitted with velocity greater than c. This suggests that the phase velocity has no physical significance and we can not respresent the wave nature of a moving particle by a single plane wave.

Group velocity:

A wave group or wave packet is described as the superposition of individual waves of different wavelengths. These waves interfere with each other and results in variation of amplitude. These defines the wave group shape. If the medium is non-dispersive, then phase velocity of the individual waves will not change with wavelength. As a result, wave packet travels with common phase velocity. But, in a dispersive medium, phase velocity of individual waves will be different. As a result, wave packet moves with a different velocity than phase velocity which is known as group velocity 'v_g'.

Let, the wave group is formed by the superposition of two monochromatic waves having same amplitude but differing in angular frequency by an amount '$\Delta\omega$' and in wave number 'Δk' i.e

$$\psi_1 = A\sin(\omega t - kx)$$

$$\psi_2 = A\sin[(\omega + \Delta\omega)t - (k + \Delta k)x]$$

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Figure : Superposition of two sinusoidal waves of slightly different frequncies [(a) and (b)] Curve (c) represents the resultant motion.

The resultant wave i.e. wave packet can be written as,

$$\psi = 2A\cos\left[\frac{1}{2}(\Delta\omega t - \Delta k x)\right]\sin(\omega t - kx)$$

Now, group velocity is the velocity with which maximum amplitude or the envelope of the wave packet moves and it is given as: $v_g = \frac{d\omega}{dk} = \frac{dE}{dp}$

From the relativistic mass-energy relation :

$$E^2 = p^2c^2 + m_0^2c^4 \qquad \Rightarrow 2E\frac{dE}{dp} = 2pc^2$$

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Therefore, $v_g = \frac{dE}{dp} = \frac{pc^2}{E} = \frac{\gamma m_0 v c^2}{\gamma m_0 c^2} = v$

Relation between Phase velocity and Group velocity: $v_g = v_p - \lambda \frac{dv_p}{d\lambda}$

For, non-dispersive medium, all waves travel with same phase velocity: $\frac{dv_p}{d\lambda} = 0 \Rightarrow v_g = v_p$

Dispersive medium are of two types:

(i) Normal dispersive medium: $\frac{dv_p}{d\lambda} = +ve \Rightarrow v_g < v_p$

(ii) Anamolous dispersive medium: $\frac{dv_p}{d\lambda} = -ve \Rightarrow v_g > v_p$

Example 15. What voltage must be applied to an electron microscope to produce electrons of wavelength 0.40Å?

Soln. De-Broglie wavelength of an electron of mass m, charge 'e' and moving under a potential of V volts is,

$$\lambda = \frac{h}{\sqrt{2meV}}$$

From the above relation, $V = 936.3$ volts

Example 16. What is the de-Broglie wavelength of an electron moving with velocity, $v = \frac{3}{5}c$?

Soln. The de-Broglie wavelength of a particle of mass 'm' moving with velocity 'v' is

$$\lambda = \frac{h}{mv} = \frac{h}{m_0 v}\sqrt{1 - v^2/c^2} = 0.0323\ A^0$$

Example 17. You have 10 eV photon and 10 eV electron. Which one has shorter wave-length?

Soln. Wavelength of photon $\lambda = \frac{hc}{E} = \frac{6.62 \times 10^{-34} \times 3 \times 10^8}{10 \times 1.6 \times 10^{-19}} = 1240\,A$

De-Broglie wavelength of the electron

$$\lambda = \frac{h}{m_0 v} = \frac{h}{\sqrt{2m_0 E}} = 3.88A^0$$

The de-Broglie wavelength λ of a particle is $\lambda \propto \frac{1}{\sqrt{E}}$ and for a photon $\lambda \propto \frac{1}{E}$. This shows that de-Broglie wavelength of an electron is much smaller as compared to that of a photon for the same energy E.

Example 18. Energy of a particle at absolute temperature T is of the order of kT. Calculate the wavelength of thermal neutrons at 27°C. [Given, the mass of the neutron $= 1.67 \times 10^{-24}\ gm$. Planck's constant, $k = 6.67 \times 10^{-27}\ erg\ \text{sec}$ and Boltzman constang, $k = 8.6 \times 10^{-5}\ eVk$]

Soln. De-Broglie wavelength of the neutron is

$$\lambda = \frac{h}{\sqrt{2mE}} = \frac{h}{\sqrt{2mkT}} = 1.78A^0$$

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Example 19. A beam of monenergetic neutrons corresponding to 27°C is allowed to fall on a crystal. A first order reflection is observed at a glancing angle 30°. Calculate the interplanar spacing of the crystal.

Given, Planck constant, $h = 6.62 \times 10^{-34}\ Js$

Mass of neutron, $m = 1.67 \times 10^{-27}\ kg$

Boltzmann constant, $k = 1.38 \times 10^{-23}\ J/K$

Soln. From Bragg law of diffraction we have,

$$2d \sin\theta = n\lambda$$

where, the glancing angle, $\theta = 30°$, order number of diffraction, n = 1

$$\therefore \quad 2d \sin 30° = \lambda,\ or,\ 2d \times \frac{1}{2} = \lambda,\ or,\ \lambda = d$$

De-Broglie wavelength of the neutron is

$$\lambda = \frac{h}{\sqrt{2mE}} = \frac{h}{\sqrt{2mkT}} = 1.78 A^0$$

Therefore, the interplanar spacing is 1.78 A^0

Example 20. What is the de-Broglie wavelength of electrons of energy 0.1 MeV using both relativistic and non-relativistic expressions for λ? What is the percentage error in using non-relativistic expression for λ?

Soln. The non-relativistic de-Broglie wavelength of an electron of mass 'm' and energy eV is,

$$\lambda_{nr} = \frac{h}{\sqrt{2meV}} = \frac{12.26}{\sqrt{V}} = \frac{12.26}{\sqrt{0.1 \times 10^6}} = 0.0388 Å$$

The relativistic expression for the de-Broglie wavelength of the same electron is,

$$\lambda_r = \frac{h}{\sqrt{2meV\left(1 + \frac{eV}{2mc^2}\right)}} = 0.0371\ A^0$$

The percentage error in using non-relativistic expression, is

$$\frac{\lambda_{nr} - \lambda_r}{\lambda_{nr}} \times 100\% = \frac{(0.0388 - 0.0371)}{0.0388} \times 100\% = 4.38\%$$

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1.4. Heisenberg's uncertainty principle :

According to classical mechanics, a moving particle has a definite momentum and position in space. Both the position and momentum of such a particle can be definitely determined. Recently, the classical view has been proved to be an approximation and is inadquate for describing the dynamical behaviour of the macroscopic objects. It cannot describe satisfactorily the behaviour of sub-atomic particles.

In quantum mechanics, a particle is described by a wave packet of linear extension (Δx) which surrounds the position of the classical particle and moves with group velocity. According to Max Born's probability interpretation, the particle may be found everywhere within the wave packet. This means that the position of the particle is uncertain within the limits (Δx) of the wave packet. So, we may say that the particle may be found anywhere within (Δx). Again, a wave packet is formed by the superposition of large number of waves having different wavelengths, the wavelength the wave packet cannot be said definitely. What we can say that the wavelength of the wave packet lies within certain range λ to $\lambda + \Delta\lambda$. As the momentum of a particle is related to wavelength by

$$p = \frac{h}{\lambda}, \Rightarrow \Delta p = -\frac{h}{\lambda^2}\Delta\lambda$$

the particle momentum is also within p to $p + \Delta p$. So, we cannot definitely say what is the momentum of the particle. Hence, because of the wave nature of partice there is uncertainty (Δx) in position of the particle as well as uncertainty in corresponding momentum (Δp).

If the number of superposed wave as well as their range of wavelength $(\Delta\lambda)$ be increased, then the linear speed (Δx) of the wave packet decreases. But simultaneously the uncertainty (Δp) in momentum increases as $\Delta p \propto \Delta\lambda$. When $\Delta\lambda = \infty, \Delta p = \infty$ and $\Delta x = 0$, i.e, the wave pocket reduces to a point. In this position, there is no uncertainty in the position of the particle.

Now for a definite $\lambda = 0, \Delta\lambda = 0$, then $\Delta p = 0 \left(\because \Delta p \propto \Delta\lambda\right)$, then there is no uncertainty in the momentum of the particle but in this case $\Delta x = \infty$, i.e., the position uncertainty is infinite since the associated wave with the particle may now extend up to ∞.

Statement of the uncertainty principle:

The uncertainty principle states that, it is fundamentally impossible to determine sumultaneously the position and the momentum of a particle to an accuracy better than one quantum of action h.

The mathematical expression of the particle is,

$$\Delta x \Delta p_x \geq \hbar$$

where, $\hbar = \frac{h}{2\pi} = 1.0545 \times 10^{-31} Js$, h being the Planck's constant $= 6.62 \times 10^{-34} Js$. Here Δx is the error (uncertainty) in the determination of position of the particle and Δp_x is the error (uncertainty) in the determination of x-component of momentum. If the position be determined accurately, then Δx becomes smaller and consequently larger is Δp_x and vice versa. It is to be kept in mind that the uncertainties are not in the appratus used for the determination but in nature itself.

In three dimensions the uncertainty relations are expressed as follows:

$$\Delta x \Delta p_x \geq \hbar; \quad \Delta y \Delta p_y \geq \hbar; \quad \Delta z \Delta p_z \geq \hbar$$

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(a) If $\Delta x = 0$, then, $\Delta p_x = \frac{\hbar}{\Delta x} \Rightarrow \Delta p_x = \frac{\hbar}{0} = \infty$

This means that, if the uncertainty in the position measurement of a moving particle be zero, then at the same moment the uncertainty in the momentum measurement will be infinity.

(b) If the momentum of a moving particle at any instant be determined accurately (i.e., $\Delta p_x = 0$), then the uncertainty (error) in the determination of position of the particle will be infinite.

(c) For a particle of mass 'm' moving with velocity v_x along the x-direction, its momentum is $p_x = mv_x$,

$$\Delta x \Delta p_x = \hbar, \quad \Delta x \Delta v_x = \frac{\hbar}{m}$$

For a heavy particle $m \to \infty$ and in that case, $\Delta x \Delta v_x = \frac{\hbar}{\infty} = 0$

For such a particle both the position and momentum can be determined accurately. This is true for macroscopic bodies whose motions are discussed in classical mechanics. Thus the uncertainty relation has no meaning in classical mechanics. But for microscopic objects such as electron, proton, atom, etc, quantum mechanics is applicable and as such the uncertainty relation is a reality in describing the dynamical behaviour of such objects.

Time-Energy Uncertainty Relation:

The time-energy uncertainty principle is stated as follows:

In any simultaneous determination of time and energy of a moving particle, the product of the uncertainties is equal to the Planck's constant,

$$\Delta E \Delta t \geq \hbar$$

Here, ΔE is the uncertainty in the measurement of energy of Δt, the corresponding uncertainty in the measurement of time.

If ΔE be the maximum uncertainty in the determination energy of a system in a particular state,then Δt is the minimum, i.e., the system remains for a minimum time in the state. On the other hand, if a system remains in a particular state for a maximum interval of time, then the uncertainty in the measurement of energy is the minimum.

Angular momentum- angular position Uncertainty Relation:

$$\Delta L.\Delta \phi \geq \hbar$$

Where, ΔL is the uncertainty in the angular momentum of the particle and $\Delta \phi$ is the uncertainty in the angular position of the particle.

Causality in Quantum Mechanics:

According to the principle of causality, knowledge of the behaviour of a system at one instant is sufficient for the prediction of its future behaviour. Thus, it is the quantum analogue of the classical principle that, the future behaviour of a particle can be determined if its position and velocity are known at a given instant. The law of causality, however, holds strictly in classical mechanics. As no observation can be made without disturbing a microsystem, it does not hold good for atomic systems.

According to Max Bron, the principle of causality can be viewed from two alternate angles. In wave-particle picture the principle of causality breaks down. But if the system be described by a wave function $\psi(\vec{r},t)$ which satisfies a differential equation of first order in time, then the behaviour of the system at a point $P(\vec{r})$ at any time 't' can be described uniquely if ψ is known at $t = 0$ at the same point $P(\vec{r})$. This shows that even for microsystems, the principle of causality is true. But the measurements on a microsystem cannot be carried out without seriously disturbing it. Hence it is impossible to determine the state of the system unambiguousy at $t = 0$. Hence it is impossible to determine the state of the system unambiguously at $t = 0$. Thus the principle of causality breaks down. Therefore, the probabilistic interpretation of the observed events are to be adopted in accordance with the uncertainty principle.

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Concept of Bohr Orbit in view of uncertainty principle:

We have the energy-time uncertainty relation, $\Delta E.\Delta t \geq \hbar$

According to the concept of Bohr, each electron revolves around the nucleus in quantised stationary orbits with definite energy E. So, the uncertainty is $\Delta E = 0$.

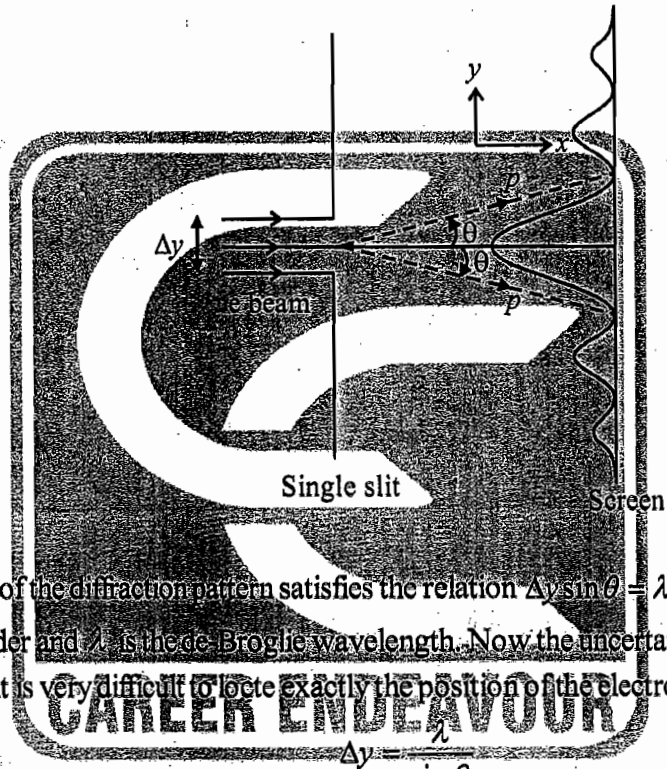
So, $$\Delta t = \frac{\hbar}{\Delta E} = \frac{\hbar}{0} = \infty$$

Hence, all energy states of the Bohr atom must have infinite lifetime $(\tau = \infty)$. This implied that radiation would not occur due to the transition of electrons. But actually $\Delta t \sim 10^{-8}$ sec leading to the occurrence of emission of radiation due to electronic transition. Thus the concept of Bohr orbit violets the Heisenberg's uncertainty principle.

Again, if Δt is finite, then $\Delta E = \frac{\hbar}{\Delta t}$ is also finite. This means that the energy levels in the excited state must have a finite spread. As a result the radiation emitted due to the transition of an electron from the excited state to the ground state is not monochromatic. This leads to the conclusion that the spectral lines can never be infinitely sharp but must have a natural broadening. This is contradiction with Bohr's theory of spectral series.

Electron difraction through a single slit:

Let a monoenergetic parallel beam of electrons moving along the x-direction be incident on a single split of width Δy. As the electron in motion is associated with de-Broglie wave, the electron beam after passing through the slit undergoes diffraction producing a fraunhofer diffraction pattern on the photoplate perpendicular to the x-axis.



The first minimum of the diffraction pattern satisfies the relation $\Delta y \sin\theta = \lambda$, where θ is the angle of diffraction for the first order and λ is the de-Broglie wavelength. Now the uncertainty in the position of an electron in the slit is Δy as it is very difficult to locte exactly the position of the electron in the slit,

$$\Delta y = \frac{\lambda}{\sin\theta}$$

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Before incidence, let the momentum of the electron along the x-direction be p. After diffraction if the electron moves along OC, then the component of momentum p along the y-direction is $p\sin\theta$. Since the electron may be anywhere within $-\theta$ to $+\theta$, the y-component of momentum must be anywhere between $-p\sin\theta$ to $p\sin\theta$.

Thus the uncertainty in the momentum measurement of the electron is,

$$\Delta p_y = p\sin\theta - (-p\sin\theta) = 2p\sin\theta = 2\frac{h}{\lambda}\sin\theta$$

Therefore, $$\Delta y \cdot \Delta py = \frac{\lambda}{\sin\theta} \times \frac{2h}{\lambda}\sin\theta = 2h \geq \hbar$$

To decrease the uncertainty in the determination position of the electron, Δy must be decreased. But the above equation shows that a decrease in Δy leads to the increase in θ and the diffraction pattern will be wider. This will cause a larger uncertainty in Δp. Thus the electron diffraction experiment established the truth of uncertainty principle.

Consequences of Heisenberg's Uncertainty principle:

(1) Non-existance of electrons within the nucleus:

Suppose electron exist within the nucleus, then uncertainty in the position of nucleus will be of the order of twice of radius of the nucleus i.e. $\Delta x = 2\times10^{-15}\,m$.

Then the minimum energy of the electron is given by

$$E_{min}^2 = p_{min}^2c^2 + m_0^2c^4 \Rightarrow E_{min} = \sqrt{(\Delta p)^2c^2 + m_0^2c^4}$$

$$\Rightarrow E_{min} = \sqrt{\left(\frac{\hbar}{2\Delta x}\right)^2 c^2 + m_0^2c^4} \approx 10MeV$$

Therefore, if electron exist within the nucleus, then minimum energy of the electron will be approximately 10 MeV. But, experimentally energy comes out to be of the order of 4 MeV. Thus, we can say that electron does not exist within the nucleus.

(2) Ground state energy of a linear harmonic oscillator:

Let a particle of mass m is executing SHM along x-axis and let at any time 't' its position is 'x' from the mean position. Therefore, $\Delta x = x$

Total energy of LHO $= E = E_K + E_P = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2 \approx \frac{(\Delta p)^2}{2m} + \frac{1}{2}m\omega^2(\Delta x)^2$

$$= \left(\frac{\hbar}{2x}\right)^2\frac{1}{2m} + \frac{1}{2}m\omega^2x^2 = \frac{\hbar^2}{8mx^2} + \frac{1}{2}m\omega^2x^2$$

For minimum energy, $\frac{dE}{dx} = -\frac{\hbar^2}{4mx^3} + m\omega^2x = 0 \Rightarrow x^2 = \frac{\hbar^2}{2m\omega}$

So, the minimum energy of the oscillator $= E_{min.} = \frac{\hbar^2}{8m}\frac{2m\omega}{\hbar} + \frac{1}{2}m\omega^2\frac{\hbar^2}{2m\omega} = \frac{1}{2}\hbar\omega$

Example 21. Assume that the uncertainty in the location of a particle is equal to its de-Broglie wavelength. Calculate the uncertainty in the velocity of the particle.

Soln. According to the uncertainty principle,

$$\Delta x\Delta p_x = \hbar \quad [\text{where } \Delta x \text{ and } \Delta p_x \text{ are the uncertainties in position and momentum}]$$

$$\Rightarrow \Delta v_x = \frac{\hbar}{m\Delta x} = \frac{\hbar}{m\lambda} \quad \left[\because \Delta x = \lambda = \frac{\hbar}{mv}\right]$$

$$= \frac{\hbar}{m\times\frac{h}{mv}} = \frac{v}{2\pi}$$

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Example 22. Suppose that the momentum of a certain particle can be measured to an accuracy of one part in 1000. Determine the minimum uncertainty in the position of the particle if the particle is (i) a $5\times10^{-3}\,kg$ mass moving with a speed of 2 m/s; (ii) an elecron moving with a speed of $1.8\times10^8\,m/s$

Soln. Given: $\frac{\Delta p}{p} = 10^{-3} \Rightarrow \Delta p = 10^{-3}p = 10^{-3}mv$

Therefore, the minimum uncertainty in position of the particle will be

$$(\Delta x)_{\min} = \frac{h}{4\pi m v \times 10^{-3}}$$

(i) $(\Delta x)_{\min} = \frac{h}{4\pi m_0 v \times 10^{-3}} = 5.28 \times 10^{-20} A^0$

(ii) $(\Delta x)_{\min} = \frac{h\sqrt{1 - v^2/c^2}}{4\pi m_0 v \times 10^{-3}} = 2.57 A^0$

Example 23. The average time interval that elapses between the excitation of an atom and the time it radiates energy is $_{10}{}^{-8}$ sec. Calculate the uncertainty in the energy of emitted photons and the limit of accuracy with which the frequency of the emitted radiation may be determined.

Soln. Uncertainty in energy of the emitted photons will be

$$\Delta E = \frac{h}{\Delta t} = 4.14 \times 10^{-7} eV$$

limit of accuracy with which the frequency of the emitted radiation may be determined will be

$$\Delta \nu = \frac{\Delta E}{h} = \frac{6.62 \times 10^{-26}}{1.6 \times 10^{-34}} = 10^8 \, cycle/sec$$

Hence, the limit of accuracy with which the frequency of the emitted radiation may be determined is $\Delta \nu = 10^8 \, Hz$.

Example 24. Find the average time that the atomic system remains in the energy state whose spectral line width is $10^{-4} \, \text{Å}$ for $\lambda = 4000 \, \text{Å}$.

Soln. From energy-time uncertainty relation, the average lifetime of the state will be

$$\Delta t = \frac{\hbar}{4\pi \Delta E} = \frac{h}{4\pi \left(\frac{hc}{\lambda^2} \Delta \lambda\right)} = \frac{\lambda^2}{4\pi c \Delta \lambda} = 4.24 \, ns$$

Example 25. In a Stern-Gerlach experiment, a collimated beam silver atom is produced by vapourising silver salt in a furnace at 1200°C. If the beam travels 100cm, use uncertainty principle to find the order of magnitude of the smallest spot that can be recorded on the detector.

[Given: Planck's constant $h = 6.6 \times 10^{-34} \, J \cdot s$; Boltzmann constant $k = 1.4 \times 10^{-23} \, J/K$. Mass of hydrogen atom $= 1.66 \times 10^{-27} \, kg$]

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Soln. If the silver atom of mass 'm' moves with velocity 'v' along the x-axis from the furnace at temperature T, then its kinetic energy is,

$$E_K = \frac{1}{2} m v^2 = \frac{3}{2} kT. \qquad \therefore v = \sqrt{\frac{3kT}{m}}$$

Time required by the silver atom to travel a distance of 100 cm is,

$$t = \frac{100}{v} = \frac{100}{\sqrt{3kT/m}}$$

Now time-energy uncertainty relation is,

$$\Delta E \Delta t \approx \hbar \Rightarrow (\Delta E)_{\min} (\Delta t)_{\max} \approx \hbar \quad \Rightarrow (\Delta E)_{\min} \approx \frac{\hbar}{(\Delta t)_{\max}} = \frac{\hbar}{t}$$

Now, $$(\Delta E_{\min})^2 = \frac{(\Delta p_{\min})^2}{2m} \Rightarrow \Delta p_{\min} = \sqrt{2mE_{\min}} = \sqrt{\frac{2m\hbar}{t}}$$

Maximum uncertainty in the position of the particle

$$(\Delta x)_{\max} \approx \frac{\hbar}{(\Delta p)_{\min}} = \sqrt{\frac{\hbar t}{2m}} = \sqrt{\frac{\hbar}{2m}} \frac{10}{\left(\frac{3kT}{m}\right)^{1/4}} = 7\times10^{-7} m = 0.7\mu m$$

The smallest spot on the detector corresponds to the maximum uncertainty in position of the silver atom. Hence, size of the smallest spot = 0.7 μm.

Example 26. The speedometer of a 180 kg vehicle reads 72 km/h at a particular instant. The readings are known to have an accuracy of ±2 km/h. What would be the minimum uncertainty in the position of the vehicle at that instant according to the Heisenberg uncertainty perinciple?

Soln. The uncertainty in the momentum is

$$\Delta p_x = \Delta(mv_x) = m\Delta v_x = (180kg)\times(2km/hr) = 100\ kg.m/s$$

Thus the minimum uncertainty in position is

$$(\Delta x)_{\min} = \frac{\hbar}{2\Delta p_x} = 0.5\times10^{-36} m$$

Remember the size of an atom is of the order of 10^{-10} m and that of a nucleus is 10^{-15}m. A size of 10^{-36} m is too small to detect with our present day technology and hence we can safely ignore it.

Example 27. Gamma rays of energy $E_0 = 14.4\ keV$ are emitted when ^{57}Fe nuclei make transition from the first excited state to the ground state. The lifetime of this excited state is about 3×10^{-8}s. If the spread in the energy of the excited state is written as $\Delta E = \frac{v}{c}E_0$, find the value of v. Here c is the speed of light in vacuum.

Soln. From energy-time uncertainty principle

$$\Delta E\Delta t \approx \hbar \Rightarrow \Delta E \approx \frac{\hbar}{\Delta t} \Rightarrow \frac{v}{c}E_0 \approx \frac{\hbar}{\Delta t}$$

$$\Rightarrow v \approx \frac{\hbar c}{E_0\tau} = \frac{hc}{2\pi E_0\tau} = \frac{1240\ eV\ nm}{2\pi\times14.4\times10^{3}\ eV} \sim 0.12\ nm/s$$

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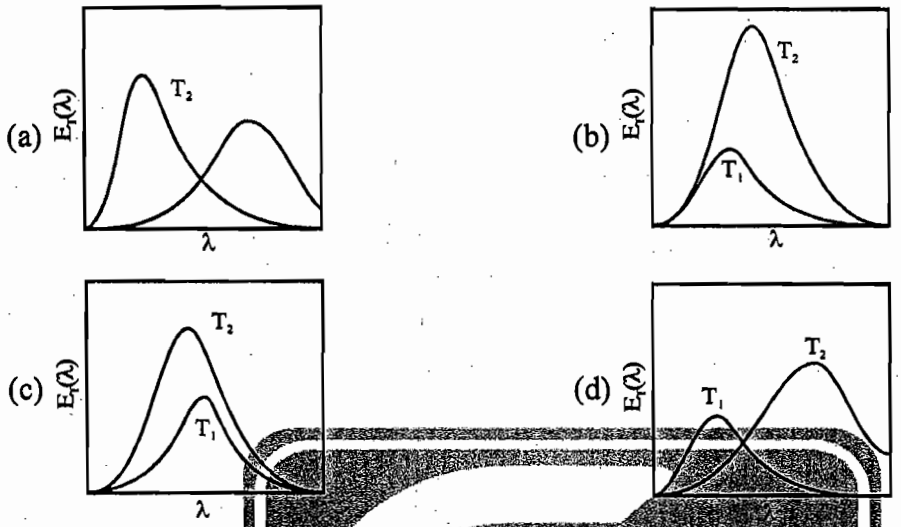
CSIR PREVIOUS YEAR QUESTIONS

Q.1. Which of the graphs below gives the correct qualitative behavior of the energy density $E_T(\lambda)$ of blackbody radiation of wavelength λ at two temperatures T_1 and T_2 $(T_1 < T_2)$? **[CSIR June 2014]**



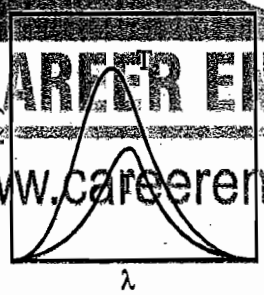
Soln. As a cosequence of Wien's displacement law, we can relate how the spectrum of black body radiation depends on the temperature of the body and corresponding mathematical equation is,

$$\lambda_m T = \text{constant}$$

where, λ_m is the wavelength at which the energy density of black body radiation, is maximum at temperature T i.e. for two temperatures T_1 and T_2

$$\frac{(\lambda_m)_1}{(\lambda_m)_2} = \frac{T_2}{T_1}$$

Since, $T_2 > T_1 \Rightarrow (\lambda_m)_1 > (\lambda_m)_2$ and the total energy density is proportional to T^4. Therefore,



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Correct answer is (c)

PRACTICE SET

1. An electron propagating along the x-axis passes through a slit of width $\Delta y = 1\ nm$. The uncertainty in the y-component of its velocity after passing through the slit is **[GATE 2002]**

(a) $7.332 \times 10^5\ m/\text{sec}$ (b) $1.166 \times 10^5\ m/\text{sec}$

(c) $3.436 \times 10^5\ m/\text{sec}$ (d) $2.326 \times 10^5\ m/\text{sec}$

2. For a free electron gas in a metal, the magnitudes of phase velocity (v_p) and group velocity (v_g) are such that **[GATE 2002]**

(a) $v_p = v_g$ (b) $v_p = \frac{1}{2} v_g$

(c) $v_p = \sqrt{2} v_g$ (d) $v_p = 2 v_g$

3. A parallel beam of electrons of a given momentum pass through a screen S_1 containing a slit and produces a diffraction pattern on a screen S_2 placed behind it. The width of the central maximum observed on the screen S_2 can be increased by **[GATE 2003]**

(a) decreasing the distance between the screen S_1 and S_2.
(b) increasing the width of the slit in screen S_1.
(c) decreasing the momentum of the electrons.
(d) increasing the momentum of the electrons.

4. Which one of the following statements concerning the compton effect is not correct? **[GATE 2003]**

(a) The wavelength of the scattered photon is greater that or equal to the wavelength of the incident photon.
(b) The electron can acquire a kinetic energy equal to the energy of the incident photon.
(c) The energy of the incident photon equals to the kinetic energy of the electron plus the energy of the scattered photon.
(d) The kinetic energy acquired by the electron is the largest when the incident and scattered photons move in opposite direction.

5. The de-Broglie wavelength for an electron of energy 150 eV is **[GATE 2005]**

(a) $10^{-8}\ m$ (b) $10^{-10}\ m$ (c) $10^{-12}\ m$ (d) $10^{-14}\ m$

6. The de Broglie wavelength of particles of mass m with average momentum p at a temperature T in three dimensions is given by **[GATE 2009]**

(a) $\lambda = \frac{h}{\sqrt{2mk_BT}}$ (b) $\lambda = \frac{h}{\sqrt{3mk_BT}}$

(c) $\lambda = \frac{h}{\sqrt{2k_BT}}$ (d) $\lambda = \frac{h}{\sqrt{2m}}$

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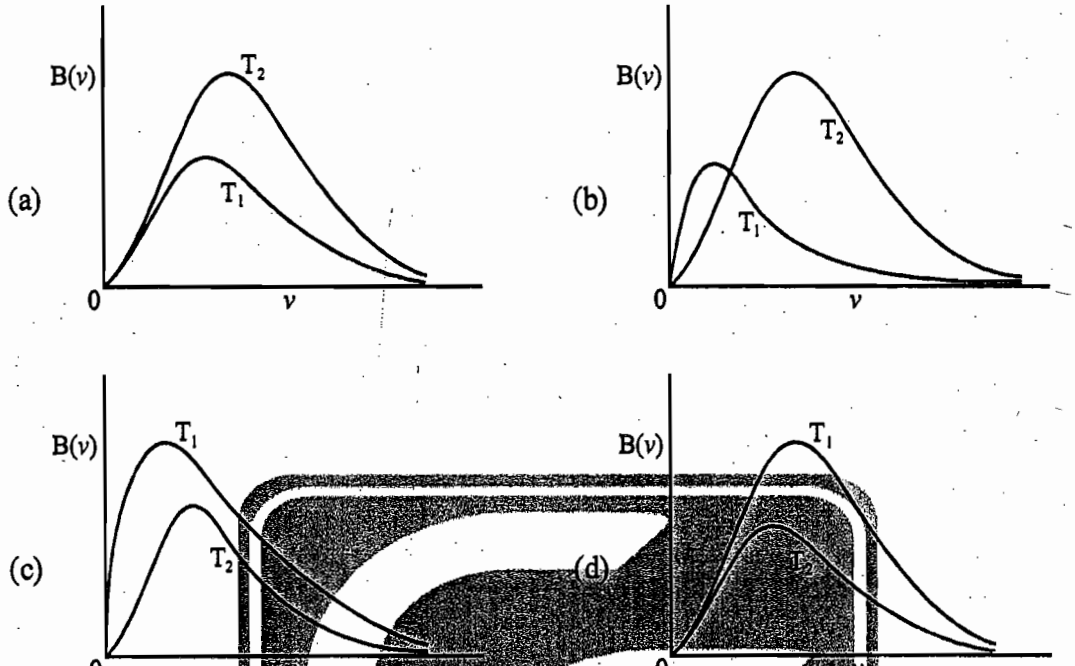
7. A proton is confined to a cubic box, whose sides have length $10^{-12}\ m$. What is the minimum kinetic energy of the proton? The mass of proton is $1.67 \times 10^{-27}\ kg$ and Planck's constant is $6.63 \times 10^{-34}\ Js$. **[GATE 2013]**

(a) $1.1 \times 10^{-17}\ J$ (b) $3.3 \times 10^{-17}\ J$

(c) $9.9 \times 10^{-17}\ J$ (d) $6.6 \times 10^{-17}\ J$

8. Two blackbodies radiate energy at temperature T_1 and T_2 $(T_1 > T_2)$. The energy emitted per unit time per unit solid angle per unit surface area of a blackbody in the frequency range ν to $\nu + d\nu$ is given by $B(\nu)d\nu$. Which one of the following graphs has the correct form? **[TIFR 2015]**



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Chapter 2

Concept of Wave Function

2.1 Introduction :

There is always a quantity asscociated with any type of waves, which varies periodically with space and time. In water waves, the quantity that varies periodically is the height of the water surface and in light waves, electric field and magnetic field vary with space and time. For De-broglie waves or matter waves asscociated with a moving particle, the quantity that vary with space and time, is called wave function of the particle.

The temporal and spatial evolution of a quantum mechanical particle is described by a wave function $\psi(x,t)$ for 1-D motion and $\psi(\vec{r},t)$ for 3-D motion. . It contains all possible information about the state of the system. These are known as configuration space wave function.

Condition for a physically accepted, well behaved, realistic wave function :

(i) $\psi(x,t)$ should be finite, single-valued and continuous everywhere in space.

(ii) $\frac{d\psi}{dx}$ should be continuous everywhere in space. But, $\frac{d\psi}{dx}$ may be discontinuous in some cases as follows:

(a) If the potential under which the particle is moving, has an infinite amount of discontinuity at some points,

(b) If the potential under which the particle is moving, is of dirac delta nature.

(iii) $\psi(x,t)$ should be square integrable i.e. $\int_{-\infty}^{\infty} |\psi(x,t)|^2 dx =$ finite quantity

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Example 1: Which of the following wave function is acceptable as the solution of the Schrodinger equation for all values of x?

(a) $\psi(x) = A\sec x$ (b) $\psi(x) = A\tan x$ (c) $\psi(x) = Ae^{x^2}$ (d) $\psi(x) = Ae^{-x^2}$

Soln. $\psi(x) = A\sec x$ and $\psi(x) = A\tan x$ is not finite at $x = \frac{\pi}{2}$.

$\psi(x) = Ae^{x^2}$ is not finite at $x = \pm\infty$; $\psi(x) = Ae^{-x^2}$ is finite everywhere in space.

Correct option is (d)

Example 2: A ball bounces back off earth. You are asked to solve this quantum mechanically assuming the earth is an infinitely hard sphere. Consider surface of earth as the origin implying $V(0) = \infty$ and a linear potential eleswhere (i.e. $V(x) = -mgx \ for \ x > 0$). Which of the following wave function is physically admissible for this problem (with $k > 0$):

(a) $\psi(x) = \frac{e^{-kx}}{x}$ (b) $\psi(x) = Ae^{-kx^2}$ (c) $\psi(x) = -Axe^{kx}$ (d) $\psi(x) = Axe^{-kx^2}$

Soln. Since the earth has been taken as infinitely hard sphere, therefore the wave function of the ball will be zero for $x<0$, non-zero for $x>0$ and zero at infinity.

Since $\psi(x)$ should be continous everywhere, the wavefunction of the ball will be zero at x = 0.

Correct option is (d).

2.2 Physical significance of wave function :

Generally, $\psi(x,t)$ is a complex quantity. It can be multipliedd by any complex number without affecting its physical significance. In general, $\psi(x,t)$ has no direct physical significance. But the quantity $\psi^*(x,t)\psi(x,t)=|\psi(x,t)|^2$ is real, physically significant and is defined as position probability density i.e. probability of finding the particle per unit length at time 't'. Therefore, for 1-D motion the probability of finding the particle between x to $x+dx$ at time 't' is given by

$$\psi^*(x,t)\psi(x,t)\,dx=|\psi(x,t)|^2\,dx$$

and for 3-D motion the probability of finding the particle within the volume element $d\tau$ located between $\vec{r}$ and $\vec{r}+d\vec{r}$ at time 't' is given by

$$\psi^*(\vec{r},t)\psi(\vec{r},t)\,d\tau=|\psi(\vec{r},t)|^2\,d\tau$$

Now, $\psi(x,t)$ or $\psi(\vec{r},t)$ should be chosen such that total probability of finding the particle in the entire space should be equal to unity i.e.

$$\int_{-\infty}^{\infty}\psi^*(x,t)\psi(x,t)\,dx=\int_{-\infty}^{\infty}|\psi(x,t)|^2\,dx=1 \text{ (for 1-D motion)}$$

$$\int_{\text{all space}}\psi^*(\vec{r},t)\psi(\vec{r},t)\,d\tau=\int_{\text{all space}}|\psi(\vec{r},t)|^2\,d\tau=1 \text{ (for 3-D motion)}$$

This is called the normalization condition of the wave function.

If $\psi(x,t)$ or $\psi(\vec{r},t)$ is normalized at some time it remains normalized forever. This can be understood as a conservation of probability or conservation of normalization.

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Method of Normalization:

Consider $\varphi(x,t)$ is an unnormalized wave function. We can construct a normalized wave function as $\psi(x,t)=N\varphi(x,t)$ where N is the normalization constant. Therefore,

$$\int_{-\infty}^{\infty}\psi^*(x,t)\psi(x,t)\,dx=|N^2|\int_{-\infty}^{\infty}\varphi^*(x,t)\varphi(x,t)dx=1$$

$$\Rightarrow N=\frac{1}{\sqrt{\int_{-\infty}^{\infty}\varphi^*(x,t)\varphi(x,t)dx}}$$

Example 3: Normalize the wave function given by

$$\psi(x)=Ne^{-\alpha x}\quad(x>0)$$

$$=Ne^{\alpha x}\quad(x<0)$$

Soln. Normalization condition is

$$\int_{-\infty}^{\infty} \psi^* \psi \, dx = 1 \Rightarrow |N|^2 \left[\int_{-\infty}^{0} e^{2\alpha x} dx + \int_{0}^{\infty} e^{-2\alpha x} dx \right] = 1$$

$$\Rightarrow |N|^2 \left[\frac{1}{2\alpha} + \frac{1}{2\alpha} \right] = 1 \quad \Rightarrow N = \sqrt{\alpha}$$

Orthogonality condition of wave functions :

Two wavefunctions $\psi_m(x)$ and $\psi_n(x)$ are said to be orthogonal to each other, if

$$\int_{-\infty}^{\infty} \psi_m^*(x) \psi_n(x) \, dx = 0 \, (m \neq n)$$

i.e. if a particle is in the state $\psi_m(x)$, then the particle cannot be in the state $\psi_n(x)$ simultaneously together.

Orthonormality condition of wave functions :

Two wavefunctions $\psi_m(x)$ and $\psi_n(x)$ are said to be orthonormal to each other, if

$$\int_{-\infty}^{\infty} \psi_m^*(x) \psi_n(x) \, dx = 0 \, (m \neq n)$$

2.3 Hilbert Space :

In a vector space , the set of unit vectors $\hat{e}_1, \hat{e}_2, \hat{e}_3$..... form the orthonormal basis i.e. we can express any vector in this vector space as a linear combination of $\hat{e}_1, \hat{e}_2, \hat{e}_3$..... Similarly, a space can be defined in which a set of functions $\phi_1(x), \phi_2(x), \phi_3(x)$..... form the orthonormal basis of the coordinate system. The corresponding infinite dimensional linear vector space is called Hilbert space.

Properties of Hilbert Space:

(i) The inner product or scalar product of two functions $\psi_i(x)$ and $\psi_j(x)$ defined in the interval $a \leq x \leq b$ is defined as

$$\langle \psi_i | \psi_j \rangle = \int \psi_i^*(x) \psi_j(x) \, dx$$

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(ii) Two functions $\psi_i(x)$ and $\psi_j(x)$ are said to be orthogonal if their inner product is zero i.e.

$$\langle \psi_i | \psi_j \rangle = \int_a^b \psi_i^*(x) \psi_j(x) \, dx = 0$$

This is known as orthogonality condition of two wave functions.

(iii) The norm of a function $\psi_i(x)$ is defined as

$$N = \sqrt{\langle \psi_i | \psi_i \rangle} = \left[\int_a^b \psi_i^*(x) \psi_i(x) \, dx \right]^{1/2}$$

(iv) A function is said to be normalized if the norm of the function is unity i.e.

$$N = \sqrt{\langle \psi_i | \psi_i \rangle} = \left[\int_a^b \psi_i^*(x) \psi_i(x) \, dx \right]^{1/2} = 1$$

This is known as normalization condition of a particular wave functions.

(v) Functions which are orthogonal and normalized are called orthonormal functions and they will satisfy the condition:

$$\langle \psi_i | \psi_j \rangle = \int_a^b \psi_i^*(x)\psi_j(x)\,dx = \delta_{ij}$$

(vi) A set of functions $\psi_1(x), \psi_2(x), \psi_3(x)$..... is linearly independent if there exist a relation like $c_1\psi_1(x) + c_2\psi_2(x) + c_3\psi_3(x) + \ldots\ldots\ldots\ldots = 0$, where all c_1, c_2, c_3..... are zero. Otherwise, they are said to be linearly dependent. A set of linearly independent functions is complete.

2.4 Operator formalism :

An operator is a mathematical rule (or procedure) which operating on one function transforms it into another function i.e. $\hat{A}\psi(x) = \phi(x)$. Every dynamical variable in Quantum mechanics represented by a operator.

Operations	Symbol	Result of the operation
Taking the square root	$\sqrt{}$	$\sqrt{x^m} = x^{m/2}$
Differentiation w.r.t. x	$\frac{d}{dx}$	$\frac{d}{dx}(x^m) = mx^{m-1}$
Position Operator :	$\hat{x}, \hat{y}, \hat{z}$	
Momentum Operator	$\hat{p}_x = -i\hbar\frac{\partial}{\partial x}$ $\hat{p}_y = -i\hbar\frac{\partial}{\partial y}$ $\hat{p}_z = -i\hbar\frac{\partial}{\partial z}$	$\Rightarrow \vec{p} = -i\hbar\vec{\nabla}$
Potential energy Operator	$\hat{V}$	
Kinetic energy Operator	$\hat{K} = \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m}\vec{\nabla}^2$	

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Commutator Bracket:

The commutator bracket of two operators $\hat{A}$ and $\hat{B}$ is defined as $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$.

Example:

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(1) $\left[\hat{x}, \frac{d}{dx}\right]\psi = \hat{x}\frac{d\psi}{dx} - \frac{d}{dx}(\hat{x}\psi) = x\frac{d\psi}{dx} - x\frac{d\psi}{dx} - \psi = -\psi \Rightarrow \left[\hat{x}, \frac{d}{dx}\right] = -1$

(2) $[\hat{x}, \hat{p}_x]\psi = \hat{x}\hat{p}_x\psi - \hat{p}_x\hat{x}\psi = -i\hbar x\frac{\partial\psi}{\partial x} + i\hbar\frac{\partial}{\partial x}(x\psi) = i\hbar\psi \Rightarrow [\hat{x}, \hat{p}_x] = i\hbar$

Similarly, $[\hat{y}, \hat{p}_y] = i\hbar$ and $[\hat{z}, \hat{p}_z] = i\hbar$

Linear Operator:

If an operator $\hat{A}$ is said to be a linear if

(i) $\hat{A}[c\psi(x)] = c\hat{A}\psi(x)$ and (ii) $\hat{A}[\psi_1(x) + \psi_2(x)] = \hat{A}\psi_1(x) + \hat{A}\psi_2(x)$

All Quantum mechanical Operators are linear in nature.

Properties of the commutator bracket:

1. $[\hat{A}, \hat{B}] = -[\hat{B}, \hat{A}]$ 2. $[\hat{A}, \hat{B} + \hat{C} + \hat{D} + \ldots.] = [\hat{A}, \hat{B}] + [\hat{A}, \hat{C}] + \ldots\ldots$

3. $\left[\hat{A},\hat{B}\right]^{\dagger}=\left[\hat{B}^{\dagger},\hat{A}^{\dagger}\right]$
4. $\left[\hat{A},\hat{B}\hat{C}\right]=\left[\hat{A},\hat{B}\right]\hat{C}+\hat{B}\left[\hat{A},\hat{C}\right]$
5. $\left[\hat{A},\left[\hat{B}\hat{C}\right]\right]+\left[\hat{B},\left[\hat{C},\hat{A}\right]\right]+\left[\hat{C},\left[\hat{A},\hat{B}\right]\right]=0$
6. $\left[\hat{A},f\left(\hat{A}\right)\right]=0$
7. $\left[f\left(\hat{A}\right),G\left(\hat{A}\right)\right]=0$
8. $\left[f\left(\hat{A}\right),G\left(\hat{B}\right)\right]=0$ only if $\left[\hat{A},\hat{B}\right]=0$
9. $\left[\hat{A},\hat{B}^{n}\right]=n\hat{B}^{n-1}\left[\hat{A},\hat{B}\right]$
10. $\left[\hat{A}^{n},\hat{B}\right]=n\hat{A}^{n-1}\left[\hat{A},\hat{B}\right]$

Example 4: Find the commutator bracket $\left[\left[\hat{A},\hat{B}\right],\left[\hat{B},\hat{A}\right]\right]$

Soln: $\left[\left[\hat{A},\hat{B}\right],\left[\hat{B},\hat{A}\right]\right]=\left[\hat{A},\hat{B}\right]\left[\hat{B},\hat{A}\right]-\left[\hat{B},\hat{A}\right]\left[\hat{A},\hat{B}\right]$

$=\left(\hat{A}\hat{B}-\hat{B}\hat{A}\right)\left(\hat{B}\hat{A}-\hat{A}\hat{B}\right)-\left(\hat{B}\hat{A}-\hat{A}\hat{B}\right)\left(\hat{A}\hat{B}-\hat{B}\hat{A}\right)$

$=\hat{A}\hat{B}\hat{B}\hat{A}-\hat{A}\hat{B}\hat{A}\hat{B}-\hat{B}\hat{A}\hat{B}\hat{A}+\hat{B}\hat{A}\hat{A}\hat{B}-\hat{B}\hat{A}\hat{A}\hat{B}+\hat{A}\hat{B}\hat{A}\hat{B}+\hat{B}\hat{A}\hat{B}\hat{A}-\hat{A}\hat{B}\hat{B}\hat{A}=0$

Example 5: Find the commutator bracket $\left[x^{2},p^{2}\right]$.

Soln: $\left[x^{2},p^{2}\right]=\left[x^{2},pp\right]=\left[x^{2},p\right]p+p\left[x^{2},p\right]=2i\hbar\left(xp+px\right)$

Example 6: If $\hat{H}=\frac{p^{2}}{2m}+V\left(x\right)$, then calculate $\left[x,\left[x,\hat{H}\right]\right]$.

Soln: $\left[x,\hat{H}\right]=\left[x,\frac{p^{2}}{2m}\right]+\left[x,V\left(x\right)\right]=\frac{1}{2m}\left[x,p^{2}\right]+0=\frac{2i\hbar p}{2m}=\frac{i\hbar}{m}p$

$\left[x,\left[x,\hat{H}\right]\right]=\left[x,\frac{i\hbar}{m}p\right]=\frac{i\hbar}{m}\left[x,p\right]=\frac{i^{2}\hbar^{2}}{m}$

Eigenvalues and Eigenfunctions:

If an operator $\hat{A}$ operating on a function $\psi_{n}(x)$ gives $\lambda\psi_{n}(x)$ i.e. $\hat{A}\psi_{n}(x)=\lambda\psi_{n}(x)$, then $\psi_{n}(x)$ is called the eigenfunction of $\hat{A}$ corresponding to eigenvalue λ and the above equation is known as eigenvalue equation of operator $\hat{A}$.

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Example: $\hat{A}=\frac{d^{2}}{dx^{2}}$ and $\psi_{n}(x)=ae^{-2x}\Rightarrow\hat{A}\psi_{n}(x)=\frac{d^{2}}{dx^{2}}\left(ae^{-2x}\right)=4ae^{-2x}=4\psi_{n}(x)$

$\psi_{n}(x)$ is an eigenfunction of $\hat{A}$ corresponding to eigenvalue 4.

If the commutator bracket of two operators $\hat{A}$ and $\hat{B}$ is equal to zero i.e. $\left[\hat{A},\hat{B}\right]=0$, then the physical observables corresponding to these operators are simultaneously accurately measurable and they have a complete set of simultaneous eigenfunctions.

Example 7: The operator $\left(x+\frac{d}{dx}\right)$ has the eigenvalue α. Determine the corresponding wavefunction.

Soln: Eigenvalue equation: $\left(x+\frac{d}{dx}\right)\psi=\alpha\psi\Rightarrow\frac{d\psi}{dx}=(\alpha-x)\psi\Rightarrow\int\frac{d\psi}{\psi}=\int(\alpha-x)dx$

$$\Rightarrow \ln\psi = \left(\alpha x - \frac{x^2}{2}\right) + \ln\psi_0 \Rightarrow \psi = \psi_0 \exp\left(\alpha x - \frac{x^2}{2}\right)$$

Example 8: Find the constant B which makes e^{-ax^2} an eigenfunction of the operator $\left(\frac{d^2}{dx^2} - Bx^2\right)$.

What is the corresponding eigenvalue?

Soln: $\left(\frac{d^2}{dx^2} - Bx^2\right)e^{-ax^2} = \left(4a^2x^2 - 2a + Bx^2\right)e^{-ax^2}$

For e^{-ax^2} to be eigenfunction of the operator $\left(\frac{d^2}{dx^2} - Bx^2\right)$, then the eigenvalue

$\left(4a^2x^2 - 2a - Bx^2\right)$ must be independent of x i.e. $\left(4a^2 - B\right) = 0 \Rightarrow B = 4a^2$

Therefore, $\left(\frac{d^2}{dx^2} - Bx^2\right)e^{-ax^2} = -2ae^{-ax^2}$. Thus the eigenvalue of the operator is (-2a).

Hermitian operator:

A operator $\hat{A}$ is said to be hermitian if $\hat{A}^\dagger = \hat{A}$ and its should satisfy the following relation:

Dirac representation: $\left\langle \phi \middle| \hat{A} \middle| \psi \right\rangle = \left\langle \psi \middle| \hat{A}^\dagger \middle| \phi \right\rangle = \left\langle \psi \middle| \hat{A} \middle| \phi \right\rangle$

Schrodinger representation: $\left(\phi, \hat{A}\psi\right) = \left(\hat{A}\phi, \psi\right) \Rightarrow \int \phi^* \hat{A}\psi\, d\tau = \int \left(\hat{A}\phi\right)^* \psi\, d\tau$

Properties:

(1) Eigenvalues of hermitian operators are real.

(2) Eigenfunctions corresponding to different eigenvalues of a hermitian operator are orthogonal.

(3) All physical observable in quantum mechanics are represented by hermitian operators.

Example: $\left(\phi, \hat{p}_x\psi\right) = \int \phi^* \left(-i\hbar\frac{\partial}{\partial x}\right)\psi\, dx = \int \phi^* \left(-i\hbar\frac{\partial\psi}{\partial x}\right) dx$

$$= -i\hbar\left[\phi^*\psi\right]_{-\infty}^{\infty} - i\hbar\int_{-\infty}^{\infty}\left(\frac{d\phi}{dx}\right)^*\psi\, dx = -i\hbar\int_{-\infty}^{\infty}\left(\frac{d\phi}{dx}\right)^*\psi\, dx = \int_{-\infty}^{\infty}\hat{p}_x^*\phi^*\psi\, dx$$

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Hence, the momentum operator $\hat{p}_x$ is hermitian in nature.

Similarly, we can see that $\frac{\partial}{\partial x}$ is anti-hermitian i.e. $\left[\frac{\partial}{\partial x}\right]^\dagger = -\frac{\partial}{\partial x}$

Projection operator:

A operator is said to be projection operator if $\hat{A}^\dagger = \hat{A}$ and $\hat{A}^2 = \hat{A}$

Properties:

(1) Eigenvalues of a projection operator is 0 and 1.

(2) Product of two projection operators is also a projection operator if $\left[\hat{p}_1, \hat{p}_2\right] = 0$

(3) Sum of two projection operator is a projection operator if $\left\{\hat{p}_1, \hat{p}_2\right\} = 0$

Unitary Operator:

An operator $\hat{A}$ is said to be unitary if $\hat{A}^{\dagger} = \hat{A}^{-1}$

Parity Opertor:

Parity opeartor corresponds to space reflection about the origin i.e $\hat{P}\psi(x) = \psi(-x)$

In general, $\hat{P}\psi(\vec{r}) = \psi(-\vec{r})$; where $\vec{r} = x\hat{i} + y\hat{j} + z\hat{k}$ and $-\vec{r} = -x\hat{i} - y\hat{j} - z\hat{k}$

When parity operator acts on a wavefunction, the following changes take place in various co-ordinate system:

(i) Cartesian co-ordinate system: $x \to -x, y \to -y, z \to -z$

(ii) Spherical polar co-ordinate system : $r \to r, \theta \to \pi - \theta, \phi \to \pi + \phi$

(iii) Cyllindrical co-ordiante system: $\rho \to \rho, \phi \to \pi + \phi, z \to -z$

Properties:

(1) Eigenvalues of the parity operator is 1, -1.

$\hat{P}\psi(x) = \psi(-x) = \psi(x) \to$ even parity. $\hat{P}\psi(x) = \psi(-x) = -\psi(x) \to$ odd parity

(2) Parity operator is hermitian in nature

(3) Parity operator commutes with hamiltonian operator if the potential under which particle is moving i.e. V(x) is symmetric in nature.

Example 9: Let, $N = \hat{b}^{\dagger}\hat{b}$ where the operator $\hat{b}$ satisfies the relation $\hat{b}\hat{b}^{\dagger} + \hat{b}^{\dagger}\hat{b} = 1$ and $\hat{b}^2 = \left(\hat{b}^{\dagger}\right)^2 = 0$; then eigenvalues of N are

(a) +ve and –ve integers (b) all +ve integers (c) –1 and 0 only (d) 0 and 1 only

Soln: $\hat{N}|\psi\rangle = \lambda|\psi\rangle \Rightarrow \hat{b}^{\dagger}\hat{b}|\psi\rangle = \lambda|\psi\rangle \Rightarrow \left(\hat{b}^{\dagger}\hat{b}\right)^2|\psi\rangle = \lambda^2|\psi\rangle$

$\Rightarrow \hat{b}^{\dagger}\hat{b}\hat{b}^{\dagger}\hat{b}|\psi\rangle = \lambda^2|\psi\rangle \Rightarrow \hat{b}^{\dagger}\left(1 - \hat{b}^{\dagger}\hat{b}\right)\hat{b}|\psi\rangle = \lambda^2|\psi\rangle$

$\Rightarrow \hat{b}^{\dagger}\hat{b} - \hat{b}^{\dagger}\hat{b}^{\dagger}\hat{b}\hat{b}|\psi\rangle = \lambda^2|\psi\rangle \Rightarrow \hat{b}^{\dagger}\hat{b}|\psi\rangle = \lambda^2|\psi\rangle \Rightarrow \lambda|\psi\rangle = \lambda^2|\psi\rangle \Rightarrow \lambda = 0, 1$

Example 10: Let the wave function of a particle of mass 'm' at a given instant be $\psi(x) = Ae^{-x^2/a^2}$.

What will be the function $K\psi(x)$ where 'K' is the kinetic energy? Is this wave function an eigenfunction of kinetic energy?

Soln. The kinetic energy operator is $K = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$. Thus,

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$$K\psi(x) = -\frac{\hbar^2}{2m}\frac{d^2}{dx}\left(Ae^{-x^2/a^2}\right) = -\frac{\hbar^2}{2m}\frac{d}{dx}\left[-\frac{2A}{a^2}xe^{-x^2/a^2}\right]$$

$$= -\frac{\hbar^2}{2m}\frac{d}{dx}\left[-\frac{2A}{a^2}xe^{-x^2/a^2}\right] = \frac{2A\hbar^2}{2ma^2}\left[x\left(\frac{-2x}{a^2}e^{-x^2/a^2}\right) + e^{-x^2/a^2}\right] = \frac{A\hbar^2}{ma^2}\left(1 - \frac{2x^2}{a^2}\right)e^{-x^2/a^2}$$

This is not an eigenfunction of kinetic energy.

Example 11: An operator A is defined as $A\psi(x) = \psi^*(x)\psi(x)$. Is this a linear operator?

Soln. For the given operator,

$$A\left[\psi_1(x) + \psi_2(x)\right] = \left[\psi_1(x) + \psi_2(x)\right]^*\left[\psi_1(x) + \psi_2(x)\right]$$

$$= \left[\psi^*{}_1(x) + \psi^*{}_2(x)\right]\left[\psi_1(x) + \psi_2(x)\right]$$

$$= \psi^*{}_1(x)\psi_1(x) + \psi^*{}_2(x)\psi_2(x) + \psi^*{}_1(x)\psi_2(x) + \psi^*{}_2(x)\psi_1(x)$$

and $A\psi_1(x)+A\psi_2(x)=\psi^*{}_1(x)\psi_1(x)+\psi^*{}_2(x)\psi_1(x)$

Thus, $A\left[\psi_1(x)+{}_2(x)\right]=\psi^*{}_1(x)+A\psi_2(x)$ and hence A is not a linear operator.

Example 12. Prove that $[Xp_x, H]=\frac{i\hbar}{m}p_x^2+X[p_x,V]$ where $H=\frac{p_x^2}{2m}+V$, and V is potential energy operator.

Soln. $[Xp_x, H]=X[p_x,H]+[X,H]p_x = X\left[p_x,\frac{p_x^2}{2m}+V\right]+\left[X,\frac{p_x^2}{2m}+V\right]p_x$

$$=X[p_x,V]+\frac{1}{2m}\left\{p_x[X,p_x]+[X,p_x]p_x\right\}p_x$$

$$=X[p_x,V]+\frac{1}{2m}(2i\hbar p_x)p_x=\frac{i\hbar}{m}p_x^2+X[p_x,V]$$

Example 13. $|\phi_1\rangle$ and $|\phi_2\rangle$ be two ortonormal state vectors. Let $A=|\phi_1\rangle\langle\phi_2|+|\phi_2\rangle\langle\phi_1|$. Is a projection operator?

Soln. $A^\dagger=\left[|\phi_1\rangle\langle\phi_2|+|\phi_2\rangle\langle\phi_1|\right]^\dagger=\left[|\phi_1\rangle\langle\phi_2|\right]^\dagger+\left[|\phi_2\rangle\langle\phi_1|\right]^\dagger=|\phi_2\rangle\langle\phi_1|+|\phi_1\rangle\langle\phi_2|=A$

Hence, A is hermitian.

Now, $A^2=\left[|\phi_1\rangle\langle\phi_2|+|\phi_2\rangle\langle\phi_1|\right]\left[|\phi_1\rangle\langle\phi_2|+|\phi_2\rangle\langle\phi_1|\right]$

$$=|\phi_1\rangle\langle\phi_2|\left[|\phi_1\rangle|\phi_2\rangle+|\phi_2\rangle\langle\phi_1|\right]+\langle\phi_2|\langle\phi_1|\left[|\phi_1\rangle\langle\phi_2|+|\phi_2\rangle\langle\phi_1|\right]$$

$$=\left[|\phi_1\rangle\langle\phi_2|\phi_1\rangle\langle\phi_2|+|\phi_1\rangle\langle\phi_2|\phi_2\rangle\langle\phi_1|\right]+\left[|\phi_2\rangle\langle\phi_1|\phi_1\rangle\langle\phi_2|+|\phi_2\rangle\langle\phi_1|\phi_2\rangle\langle\phi_1|\right]$$

Since, $|\phi_1\rangle$ and $|\phi_2\rangle$ are orthonormal,

$$A^2=|\phi_1\rangle\langle\phi_2|+|\phi_2\rangle\langle\phi_1|=A$$

Therefore, A is not a projection operator.

Example 14. Prove that $\frac{d}{dt}\langle x^2\rangle=\frac{1}{m}\langle Xp_x+p_xX\rangle$

Soln. $\frac{d}{dt}\langle x^2\rangle=\frac{1}{i\hbar}\left\langle\left[X^2,H\right]\right\rangle=\frac{1}{i\hbar}\left\langle\left[X^2,\frac{p_x^2}{2m}+V(x)\right]\right\rangle$

$$=\frac{1}{2mi\hbar}\left\langle\left[X^2,p_x^2\right]\right\rangle=\frac{1}{2mi\hbar}\left\langle p_x\left[X^2,p_x\right]+\left[X^2,p_x\right]p_x\right\rangle$$

$$=\frac{1}{2mi\hbar}\left\langle p_x(2i\hbar X)+(2i\hbar X)p_x\right\rangle=\frac{1}{m}\langle p_xX+Xp_x\rangle=\frac{1}{m}\langle Xp_x+p_xX\rangle$$

Example 15. Prove that the operators $i(d/dx)$ and d^2/dx^2 are Hermitian.

Soln. $\int_{-\infty}^{\infty}\psi_m^*\left(i\frac{d}{dx}\right)\psi_n dx=i[\psi_m^*\psi_n]_{-\infty}^{\infty}-i\int_{-\infty}^{\infty}\psi_n\frac{d}{dx}\psi_m^* dx \quad =\int_{-\infty}^{\infty}\left(i\frac{d}{dx}\psi_m\right)^*\psi_n dx$

Therefore, id/dx is Hermitian.

$$\int_{-\infty}^{\infty}\psi_m^*\frac{d^2\psi_n}{dx^2}dx=\left[\psi_m^*\frac{d\psi_n}{dx}\right]_{-\infty}^{\infty}-\int_{-\infty}^{\infty}\frac{d\psi_n}{dx}\frac{d\psi_m^*}{dx}dx$$

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$$= \left[\frac{d\psi_m^*}{dx}\psi_n\right]_{-\infty}^{\infty} + \int_{-\infty}^{\infty}\psi_n\frac{d^2\psi_m^*}{dx^2}dx = \int_{-\infty}^{\infty}\frac{d^2\psi_m^*}{dx^2}\psi_n dx$$

Thus, d^2/dx^2 is Hermitian.

Example 16: Find the following commutation relations:

(i) $\left[\frac{\partial}{\partial x}, \frac{\partial^2}{\partial x^2}\right]$ (ii) $\left[\frac{\partial}{\partial x}, F(x)\right]$

Soln. (i) $\left[\frac{\partial}{\partial x}, \frac{\partial^2}{\partial x^2}\right]\psi = \left(\frac{\partial}{\partial x}\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial x^2}\frac{\partial}{\partial x}\right)\psi = \left(\frac{\partial^3}{\partial x^3} - \frac{\partial^3}{\partial x^3}\right)\psi = 0$

(iii) $\left[\frac{\partial}{\partial x}, F(x)\right]\psi = \frac{\partial}{\partial x}(F\psi) - F\frac{\partial}{\partial x}\psi = \frac{\partial F}{\partial x}\psi + F\frac{\partial\psi}{\partial x} - F\frac{\partial\psi}{\partial x} = \frac{\partial F}{\partial x}\psi$

Thus, $\left[\frac{\partial}{\partial x}, F(x)\right] = \frac{\partial F}{\partial x}$

Example 17: Find the equivalence of the following operators:

(i) $\left(\frac{d}{dx}+x\right)\left(\frac{d}{dx}+x\right)$ (ii) $\left(\frac{d}{dx}+x\right)\left(\frac{d}{dx}-x\right)$

Soln. (i) $\left(\frac{d}{dx}+x\right)\left(\frac{d}{dx}+x\right)\psi(x) = \left(\frac{d}{dx}+x\right)\left(\frac{d\psi}{dx}+x\psi\right)$

$$= \frac{d^2\psi}{dx^2} + x\frac{d\psi}{dx} + \psi + x\frac{d\psi}{dx} + x^2\psi = \left(\frac{d^2}{dx^2} + 2x\frac{d}{dx} + x^2 + 1\right)\psi$$

Therefore, $\left(\frac{d}{dx}+x\right)\left(\frac{d}{dx}+x\right) = \frac{d^2}{dx^2} + 2x\frac{d}{dx} + x^2 + 1$

(ii) Similarly, $\left(\frac{d}{dx}+x\right)\left(\frac{d}{dx}-x\right) = \frac{d^2}{dx^2} - x^2 - 1$

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Example 18. By what factors do the operators $(x^2p_x^2 + p_x^2x^2)$ and $1/2(xp_x + p_xx)^2$ differ?

Soln. $(x^2p_x^2 + p_x^2x^2)f = -\hbar^2\left[x^2\frac{\partial^2 f}{\partial x^2} + \frac{\partial^2(x^2f)}{\partial x^2}\right]$

$$= -\hbar^2x^2\frac{\partial^2 f}{\partial x^2} - \hbar^2\frac{\partial}{\partial x}\frac{\partial(x^2f)}{\partial x} = -\hbar^2x^2\frac{\partial^2 f}{\partial x^2} - \hbar^2\frac{\partial}{\partial x}\left(2xf + x^2\frac{\partial f}{\partial x}\right)$$

$$= -\hbar^2\left(x^2\frac{\partial^2 f}{\partial x^2} + 2f + 2x\frac{\partial f}{\partial x} + x^2\frac{\partial^2 f}{\partial x^2} + 2x\frac{\partial f}{\partial x}\right) = -\hbar^2\left(2x^2\frac{\partial^2}{\partial x^2} + 4x\frac{\partial}{\partial x} + 2\right)f$$

$$\frac{1}{2}(xp_x + p_xx)^2 f = -\frac{i\hbar}{2}(xp_x + p_xx)\left[x\frac{\partial f}{\partial x} + \frac{\partial(xf)}{\partial x}\right]$$

$$= -\frac{i\hbar}{2}(xp_x + p_x x)\left(2x\frac{\partial f}{\partial x} + f\right)$$

$$= -\frac{\hbar^2}{2}\left[x\frac{\partial}{\partial x}\left(2x\frac{\partial f}{\partial x}\right) + x\frac{\partial f}{\partial x} + \frac{\partial}{dx}\left(2x^2\frac{\partial f}{\partial x}\right) + \frac{\partial(xf)}{\partial x}\right]$$

$$= -\frac{\hbar^2}{2}\left(2x^2\frac{\partial^2 f}{\partial x^2} + 2x\frac{\partial f}{\partial x} + x\frac{\partial f}{\partial x} + 2x^2\frac{\partial^2 f}{\partial x^2} + 4x\frac{\partial f}{\partial x} + x\frac{\partial f}{\partial x} + f\right)$$

$$= -\frac{\hbar^2}{2}\left(8x\frac{\partial f}{\partial x} + 2x^2\frac{\partial^2 f}{\partial x^2} + f\right) = -\hbar^2\left(2x^2\frac{\partial^2}{\partial x^2} + 4x\frac{\partial}{\partial x} + \frac{1}{2}\right)f$$

The two operators differ by a term $-(3/2)\hbar^2$

Example 19. Find the eigenvalues and eigenfunctions of the operator d/dx.

Soln. Eigenvalue equation: $\frac{d}{dx}\psi(x) = k\psi(x)$ (where k is the eigenvalue and $\psi(x)$ is the eigenfunction)

$$\Rightarrow \frac{d\psi}{\psi} = kdx \quad \Rightarrow \psi = Ce^{kx}$$

Case 1: k is a real positive quantity, ψ is not an acceptable function since it tends to ∞ or $-\infty$ as $x \to \infty$ or $-\infty$.

Case 2: k is purely imaginary (say ia), then $\psi = Ce^{iax}$ which will be finite for all values of x.

Hence, $y = ce^{kx}$ is the eigenfunction of the operator d/dx with eigenvalues $k = ia$, where a is real.

Expectation value of dynamic variables:

It is defined as the average of the result of a large number of independent measurements of a physical observable on the same system.

$$\langle \hat{A} \rangle = \frac{\int_{-\infty}^{\infty} \psi^* \hat{A} \psi dx}{\int_{-\infty}^{\infty} \psi^* \psi dx} = \frac{\langle \psi | \hat{A} | \psi \rangle}{\langle \psi | \psi \rangle}$$

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Note:

(1) If the state of the particle is an eigenfunction of the operator $\hat{A}$, then the expectation value of the physical observable corresponding to $\hat{A}$ will be equal to the eigenvalue of $\hat{A}$ corresponding to the state of the particle.

(2) The state of the particle is given as:

$$|\psi\rangle = C_1|\phi_1\rangle + C_2|\phi_2\rangle + C_3|\phi_3\rangle + \ldots\ldots\ldots\ldots = \sum_n C_n|\phi_n\rangle$$

where $|\phi_1\rangle, |\phi_2\rangle$..... are the eigenfunction of the operator $\hat{A}$, then expectation value of the the physical observable corresponding to $\hat{A}$ will be

$$\langle \hat{A} \rangle = \sum_n |C_n|^2 \lambda_n$$

where λ_n are the eigenvalues of operator $\hat{A}$ corresponding to $|\phi_n\rangle$

Example 20: A particle of mass 'm' is confined in a 1-D box from $x=-2L$ to $x=2L$. The wave function of the particle in this state is $\psi(x)=\psi_0\cos\left(\frac{\pi x}{4L}\right)$

(i) Find the normalization factor.
(ii) The expectation value of P^2 in this state.

Soln. (i) $\int_{-\infty}^{\infty}\psi^*\psi\,dx=1 \Rightarrow |\psi_0|^2\int_{-2L}^{2L}\cos^2\left(\frac{\pi x}{4L}\right)dx=1 \Rightarrow |\psi_0|^2\int_{-2L}^{2L}\frac{1}{2}\left(1+\cos\frac{2\pi x}{4L}\right)dx$

$$\Rightarrow \frac{|\psi_0|^2}{2}\left[x-\sin\left(\frac{2\pi x}{4L}\right)\times\frac{4L}{2\pi}\right]_{-2L}^{+2L}=1 \Rightarrow \frac{|\psi_0|^2}{2}\left[(2L+2L)\right]=1 \Rightarrow |\psi_0|=\frac{1}{\sqrt{2L}}$$

$$\langle P^2\rangle=\int_{-2L}^{2L}\psi^*\left[-\hbar^2\frac{d^2}{dx^2}\right]\psi\,dx = =\frac{\hbar^2}{2L}\int_{-2L}^{2L}\cos^2\left(\frac{\pi x}{4L}\right)\left(\frac{\pi}{4L}\right)^2dx$$

$$=\frac{\hbar^2}{2L}\cdot\frac{\pi^2}{16L^2}\frac{1}{2}\int_{-2L}^{+2L}\left(1+\cos\frac{\pi x}{2L}\right)dx=\frac{\pi^2\hbar^2}{32L^3}\int_0^{2L}\left(1+\cos\frac{\pi x}{2L}\right)dx=\frac{\pi^2\hbar^2}{16L^2}$$

Example 21: Find the expected value of position and momentum of a particle whose wave function is $\psi(x)=e^{-x^2/a^2+ikx}$ in all space

Soln. Expected position of the particle $\langle x\rangle=\frac{\int_{-\infty}^{\infty}\psi^*x\psi\,dx}{\int_{-\infty}^{\infty}\psi^*\psi\,dx}=\frac{\int_{-\infty}^{\infty}e^{-2x^2/a^2}x\,dx}{\int_{-\infty}^{\infty}e^{-2x^2/a^2}dx}=0$

Expected momentum of the particle

$$\langle p\rangle=\frac{\int_{-\infty}^{\infty}e^{-x^2/a^2-ikx}\left(-i\hbar\frac{\partial}{\partial x}\right)e^{-x^2/a^2+ikx}dx}{\int_{-\infty}^{\infty}e^{-2x^2/a^2}dx}=\frac{\int_{-\infty}^{\infty}e^{-2x^2/a^2}\left(-\frac{2x}{a^2}+ik\right)dx}{\int_{-\infty}^{\infty}e^{-2x^2/a^2}dx}=\hbar k\frac{\int_{-\infty}^{\infty}e^{-2x^2/a^2}dx}{\int_{-\infty}^{\infty}e^{-2x^2/a^2}dx}=\hbar k$$

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Example 22. The wavefunction of a particle in a state is $\psi=N\exp(-x^2/2\alpha)$, where $N=(1/\pi\alpha)^{1/4}$. Evaluate $(\Delta x)(\Delta p)$.

Soln. Since ψ is symmetrical about $x=0, \langle x\rangle=0$

$$\langle x^2\rangle=N^2\int_{-\infty}^{\infty}x^2\exp\left(\frac{-x^2}{\alpha}\right)dx=\frac{\alpha}{2}$$

Since, ψ is a real wave function, $\langle p\rangle=0$

$$\langle p^2\rangle=(-i\hbar)^2N^2\int_{-\infty}^{\infty}\exp\left(\frac{-x^2}{2\alpha}\right)\frac{d^2}{dx^2}\exp\left(\frac{-x^2}{2\alpha}\right)dx$$

$$=\frac{\hbar^2N^2}{\alpha}\int_{-\infty}^{\infty}\exp\left(\frac{-x^2}{\alpha}\right)dx-\frac{\hbar^2N^2}{\alpha^2}\int_{-\infty}^{\infty}x^2\exp\left(\frac{-x^2}{\alpha}\right)dx$$

$$= \frac{\hbar^2}{\alpha} - \frac{\hbar^2}{2\alpha} = \frac{\hbar^2}{2\alpha}$$

Therefore, $\Delta x \Delta p = \left[\sqrt{\langle x^2\rangle - \langle x\rangle^2}\right]\left[\sqrt{\langle p^2\rangle - \langle p\rangle^2}\right] = \sqrt{\frac{\alpha}{2}}\sqrt{\frac{\hbar^2}{2\alpha}} = \frac{\hbar}{2}$

Example 23. The Hamiltonian operator of a system is $H = -(d^2/dx^2) + x^2$. Show that $Nx\exp(-x^2/2)$ is an eigenfunction of H and determine the eigenvalue. Also evaluate N by normalization of the function.

Soln. $\psi = Nx\exp(-x^2/2), N$ being a constant

$$H\psi = \left(-\frac{d^2}{dx^2} + x^2\right) Nx\exp\left(-\frac{x^2}{2}\right) = Nx^3\exp\left(-\frac{x^2}{2}\right)\frac{d}{dx}\left[\exp\left(-\frac{x^2}{2}\right) - x^2\exp\left(-\frac{x^2}{2}\right)\right]$$

$$= 3Nx\exp\left(-\frac{x^2}{2}\right) = 3\psi$$

Thus, the eigenvalue of H is 3. The normalization condition gives

$$N^2\int_{-\infty}^{\infty} x^2 e^{-x^2}dx = 1 \Rightarrow N^2\frac{\sqrt{\pi}}{2} = 1 \Rightarrow N = \left(\frac{2}{\sqrt{\pi}}\right)^{1/2}$$

The normalized function $\psi = \left(\frac{2}{\sqrt{\pi}}\right)^{1/2} x\exp\left(-\frac{x^2}{2}\right)$

Example 24. Consider the wave function $\psi(x) = A\exp\left(-\frac{x^2}{a^2}\right)\exp(ikx)$, where A is a real constant.

(i) Find the value of A. (ii) calculate $\langle p\rangle$ for this wave function.

Soln. (i) Normalization condition: $A^2\int_{-\infty}^{\infty}\exp\left(-\frac{2x^2}{a^2}\right)dx = 1$

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$$\Rightarrow A^2\left(\frac{\pi}{2/a^2}\right)^{1/2} = 1 \quad \Rightarrow A = \sqrt{\frac{2}{\pi}}a$$

(ii) $\langle p\rangle = \int\psi^*\left(-i\hbar\frac{d}{dx}\right)\psi dx = (-i\hbar)A^2\int_{-\infty}^{\infty}\exp\left(-\frac{x^2}{a^2}\right)e^{-ikx}\left(-\frac{2x}{a^2} + ik\right)\exp\left(-\frac{x^2}{a^2}\right)e^{-ikx}dx$

$$= (-i\hbar)\left(-\frac{2}{a^2}\right)\int_{-\infty}^{\infty}\exp\left(\frac{-2x^2}{a^2}\right)xdx + (-i\hbar)(ik)A^2\int_{-\infty}^{\infty}\exp\left(\frac{-2x^2}{a^2}\right)dx$$

In the first term, the integrand is odd and the integral is from $-\infty$ to ∞. Hence the integral vanishes.

Therefore, $\langle p\rangle = \hbar k$, since $A^2\int_{-\infty}^{\infty}\exp\left(\frac{-2x^2}{a^2}\right)dx = 1$

Example 25. The normalized wave function of a particle is $\psi(x) = A\exp(iax - ibt)$, where A, a and b are constants. Evaluate the uncertainty in its momentum.

Soln. $\langle p \rangle = -i\hbar \int \psi^* \frac{d}{dx}\psi dx = \hbar a \int \psi^* \psi dx = \hbar a$

$$\langle p^2 \rangle = -\hbar^2 \int \psi^* \frac{d^2}{dx^2}\psi dx = -\hbar^2 (ia)^2 \int \psi^* \psi \, dx = \hbar^2 a^2$$

Uncertainty in mometum $(\Delta p) = \sqrt{\langle p^2 \rangle - \langle p \rangle^2} = \sqrt{\hbar^2 a^2 - \hbar^2 a^2} = 0$

Example 26: A particle of mass 'm' is subjected to the potential energy $V(x) = \frac{1}{2}kx^2$. At a particular time, it has the wave function $\psi(x) = Axe^{-x^2/a^2}$. If the particle has a definite total mechanical energy, find the value of 'a'.

Soln. The operator corresponding to the total mechanical energy is $H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$. If the particle has definite vlaue of the total mechanical energy, its wave function should be an eigenfunction of H, that is,

$H\psi(x) = \lambda\psi(x)$ where λ is independent of x.

$$H\psi(x) = \left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}kx^2\right]\left[Axe^{-x^2/a^2}\right]$$

$$= -\frac{A\hbar^2}{2m}\frac{d^2}{dx^2}\left(xe^{-x^2/a^2}\right) + \frac{1}{2}kAx^3e^{-x^2/a^2}$$

$$= -\frac{A\hbar^2}{2m}\frac{d}{dx}\left[\left(1 - \frac{2x^2}{a^2}\right)e^{-x^2/a^2}\right] + \frac{1}{2}kAx^3e^{-x^2/a^2}$$

$$= -\frac{A\hbar^2}{2m}\left[\left(-\frac{2x}{a^2} - \frac{2x}{a^2}\right) + \left(\frac{4x^2}{a^4} - \frac{2}{a^2}\right)\right]e^{-x^2/a^2} + \frac{1}{2}kAx^3e^{-x^2/a^2}$$

$$= -\frac{A\hbar^2}{2m}\left[-\frac{6x}{a^2} + \frac{4x^3}{a^4}\right]e^{-x^2/a^2} + \frac{1}{2}kAx^3e^{-x^2/a^2}$$

$$= \frac{3A\hbar^2}{ma^2}xe^{-x^2/a^2} - \left(\frac{2A\hbar^2}{ma^4} - \frac{1}{2}kA\right)x^3e^{-x^2/a^2}$$

If $H\psi(x)$ has to have the same functional form as $\psi(x)$, one should not have the $x^3e^{-x^2/a^2}$ term. So,

$$\frac{2A\hbar^2}{ma^4} - \frac{1}{2}kA = 0 \quad \Rightarrow a = \left[\frac{4\hbar^2}{mk}\right]^{1/4}$$

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Example 27. A particle moves in a linear potential $V(x) = -kx$, (i.e. under a constant force condition). Show that $\langle x \rangle$ follows rigorously the same time evolution as given by Newton's laws.

Soln. The equation for $\langle x \rangle$ is

$$\frac{d^2}{dt^2}\langle x \rangle = \frac{1}{m}\left\langle -\frac{dV}{dx} \right\rangle$$

As $V(x) = -kx, -\frac{dV}{dx} = k$ which is independent of 'x' and equals the force in classical physics. The expectation value $\left\langle -\frac{dV}{dx} \right\rangle$ is also equal to because $-\frac{dV}{dx}$ is independent of 'x'. Thus

$$\frac{d^2}{dt^2}\langle x \rangle = \frac{k}{m} = \frac{F}{m}$$

According to the Newton's law, the position 'x' of the particle moves in accordance with the equation $\frac{d^2x}{dt^2} = \frac{F}{m}$.

So, $\langle x \rangle$ evolves in the time rigorously the same way as 'x' evolves in classical physics

2.5 Schrodinger Equation :

Consider a particle of mass 'm' is moving along x axis, under the potential field $V(x)$ which is independent of time. The total energy of the system can be written as

$$E = E_k + E_p = \frac{p_x^2}{2m} + V(x)$$

Now, the 1-D time-dependent Schrodinger equation for the system can be written as

$$\hat{H}\psi = \hat{E}\psi \quad \Rightarrow -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi = i\hbar\frac{\partial\psi}{\partial t}$$

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Solution of 1-D time-dependent Schrodinger equation:

Let, $\psi(x,t) = X(x)T(t)$

Replecing this in the 1-D time-dependent Schrodinger equation

$$\Rightarrow -\frac{\hbar^2}{2m}T\frac{\partial^2 X}{\partial x^2} + VXT = i\hbar X\frac{\partial T}{\partial t}$$

$$\Rightarrow -\frac{\hbar^2}{2m}\frac{1}{X}\frac{d^2X}{dx^2} + V = \frac{i\hbar}{T}\frac{dT}{dt} = E \text{ (constant)}$$

Time dependent part:

$$i\hbar\frac{1}{T}\frac{\partial T}{\partial t} = E \quad \Rightarrow \frac{\partial T}{T} = \frac{E}{i\hbar}\partial t = -\frac{i}{\hbar}Edt$$

$$\Rightarrow T(t) = Ce^{-i\frac{E}{\hbar}t}$$

Therefore, the time dependent part of the solution of the 1-D Schrodinger equation is independent of $V(x)$.

Time independent part:

$$-\frac{\hbar^2}{2m}\frac{1}{X}\frac{\partial^2 X}{\partial x^2}+V=E \Rightarrow -\frac{\hbar^2}{2m}\frac{d^2X}{dx^2}+VX=EX$$

$$\Rightarrow \frac{d^2X}{dx^2}+\frac{2m}{\hbar^2}\left[E-V(x)\right]X=0$$

Therefore, the time independent part of the solution of the 1-D schrodinger equation depends on the nature of $V(x)$.

So, the solution of the 1-D time dependent Schrodinger equation can be written as

$$\psi(x,t)=X(x)T(t)=X(x)e^{-iEt/\hbar}$$

Now, if $\psi_1(x,t),\psi_2(x,t).....\psi_n(x,t)$ are solutions of 1-D time dependent Schrodinger equation corre sponding to energies $E_1, E_2, E_3,.....E_n$, then the general solution is

$$\psi(x,t)=\psi_1(x,t)+\psi_2(x,t)+.....$$
$$=C_1X_1(x)e^{-iE_1t/\hbar}+C_2X_2e^{-iE_2t/\hbar}+C_3X_3e^{-iE_3t/\hbar}+.....=\sum_n C_nX_n(x)e^{-iE_nt/\hbar}$$

Example 28: The wave function of a spinless particle of mass 'm' is 1-D potential is $\psi(x)=A\exp\left(-\alpha^2x^2\right)$, corresponding to eigenvalue $E_0=\frac{\hbar^2\alpha^2}{m}$. The potential $V(x)$ is

(a) $2E_0\left(1-\alpha^2x^2\right)$ (b) $2E_0\left(1+\alpha^2x^2\right)$ (c) $2E_0\alpha^2x^2$ (d) $2E_0\alpha^2x^2\left(1+2\alpha^2x^2\right)$

Soln. Given: $\psi(x)=A\exp\left(-\alpha^2x^2\right) \Rightarrow \frac{\partial\psi}{\partial x}=A\exp\left(-\alpha^2x^2\right)\left(-2\alpha^2x\right)$

$$\Rightarrow \frac{\partial^2\psi}{\partial x^2}=A\exp\left(-\alpha^2x^2\right)\left(4\alpha^4x^2\right)+A\exp\left(-\alpha^2x^2\right)\left(-2\alpha^2\right)$$

Replacing all these in the 1-D time independent Schrodinger equation i.e

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}+V(x)\psi=E\psi$$

we get

$$\Rightarrow -\frac{\hbar^2}{2m}\left[A\exp\left(-\alpha^2x^2\right)\left(4\alpha^4x^2\right)\right]+A\exp\left(-\alpha^2x^2\right)V(x)+A\exp\left(-\alpha^2x^2\right)\left(-2\alpha^2\right)=E.A\exp\left(-\alpha^2x^2\right)$$

$$\Rightarrow -\frac{\hbar^2}{2m}\left[4\alpha^4x^2-2\alpha^2\right]+V(x)=E \Rightarrow V(x)-\frac{\hbar^2}{2m}4\alpha^4x^2+\frac{\hbar^2\alpha^2}{m}=\frac{\hbar^2\alpha^2}{m}$$

Therefore, $V(x)=\frac{2\alpha^4\hbar^2x^2}{m}=2E_0\alpha^2x^2$

Example 29: The wave function of a particle moving in a 1-D potential $V(x)$ is $\psi(x)=\exp(-iax+b)$. The potential $V(x)$ will be the form:

(a) $V(x)\propto x^2$ (b) $V(x)\propto x$ (c) $V(x)=0$ (d) $V(x)\propto e^{-ax}$

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Soln. $-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}+V\psi=E\psi \Rightarrow -\frac{\hbar^2}{2m}a^2+V(x)=E \qquad \Rightarrow V(x)=0$

Correct option is (c).

Example 30: The ground state (a part from normalization) of a particle moving in a 1-D potential given by, $\psi(x)=\exp\left(-\frac{x^2}{2}\right)\cosh\left(\sqrt{2}x\right)$. The potential $V(x)$ is (taking m = 1, $\hbar=1$)

(a) $\frac{x^2}{2}$ (b) $\frac{x^2}{2}-\sqrt{2}\tanh\left(\sqrt{2}x\right)$ (c) $\frac{x^2}{2}-\sqrt{2}\tan\left(\sqrt{2}x\right)$ (d) $\frac{x^2}{2}-\coth\left(\sqrt{2}x\right)$

Soln. Given: $\psi=\exp\left(-\frac{x^2}{2}\right)\cosh\left(\sqrt{2}x\right)$

$$\psi'=\exp\left(-\frac{x^2}{2}\right)(-x)\cosh\left(\sqrt{2}x\right)+\exp\left(-\frac{x^2}{2}\right)\sqrt{2}\sinh\sqrt{2}x$$

$$\psi''=\exp\left(-\frac{x^2}{2}\right)(x^2)\cosh\left(\sqrt{2}x\right)-\exp\left(-\frac{x^2}{2}\right)\cosh\sqrt{2}x-\sqrt{2}x\exp\left(-\frac{x^2}{2}\right)\sinh\left(\sqrt{2}x\right)$$

$$+\exp\left(-\frac{x^2}{2}\right)(-x)\sqrt{2}\sinh\sqrt{2}x+\exp\left(-\frac{x^2}{2}\right)2\cosh\sqrt{2}x$$

Replacing all these in the 1-D time independent Schrodinger equation, i.e

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}+V(x)\psi=E\psi$$

we get

$$\Rightarrow -\frac{\hbar^2}{2m}\left[x^2\cosh\left(\sqrt{2}x\right)-\cosh\sqrt{2}x-\sqrt{2}x\right]\sinh\sqrt{2}x-x\sqrt{2}\sinh\sqrt{2}x$$

$$+2\cosh\sqrt{2}x+V\cosh\left(\sqrt{2}x\right)=E\cosh\left(\sqrt{2}x\right)$$

$$\Rightarrow -\frac{\hbar^2}{2m}\left[x^2-1-2\sqrt{2}x\tanh\left(\sqrt{2}x\right)+2\right]+V=E$$

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Since, energy of the particle E is independent of x, then

$$\Rightarrow V(x)-\frac{\hbar^2}{2m}\left(x^2-2\sqrt{2}\tanh\left(\sqrt{2}x\right)\right)=0 \Rightarrow V(x)=\frac{\hbar^2}{2m}\left(x^2-2\sqrt{2}\tanh\left(\sqrt{2}x\right)\right)$$

Taking $m=1,\hbar=1$ we get, $\Rightarrow V(x)=\frac{x^2}{2}-\sqrt{2}\tanh\left(\sqrt{2}x\right)$

Superposition of States:

If $|\phi_1\rangle,|\phi_2\rangle,|\phi_3\rangle.....|\phi_n\rangle$ are orthonormal state vectors/wave functions and are representing state of quantum mechanics system. then any linear combination will also represent state of a quantum mechanics system. In other words, if $\phi_1,\phi_2,.....\phi_n$ are solutions of Schrodinger equation, then linear combination/superposition of the states i.e.

$$|\psi\rangle = C_1|\phi_1\rangle + C_2|\phi_2\rangle + C_3|\phi_3\rangle + \ldots\ldots\ldots\ldots = \sum_n C_n|\phi_n\rangle$$

will also be a solution of Schrodinger equation.

Note:

(1) $|\psi\rangle$ will be normalized if $|C_1|^2 + |C_2|^2 + |C_3|^2 \ldots\ldots\ldots\ldots = 1$

(2) Probability of finding a particle in $|\phi_1\rangle$ state $= |C_1|^2 = |\langle\phi_1|\psi\rangle|^2$

Example 31: Consider a system whose initial state at t = 0 is given in terms of 3 orthonormal state vectors $|\phi_1\rangle, |\phi_2\rangle, |\phi_3\rangle$ as

$$|\psi(x,0)\rangle = \frac{1}{\sqrt{2}}|\phi_1\rangle + A|\phi_2\rangle + \frac{1}{\sqrt{5}}|\phi_3\rangle \qquad \text{(A is a real constant)}$$

(i) Find the value of A so that $|\psi(x,0)\rangle$ is normalized.

(ii) What are probabilities regarding the system to be in $|\phi_1\rangle, |\phi_2\rangle, |\phi_3\rangle$ states.

(iii) Find the state of the system at any time 't'.

Soln. (i) Normalization condition:

$$\langle\psi|\psi\rangle = 1 \quad \Rightarrow \sum C_n^2 = 1 \quad \Rightarrow \frac{1}{2} + A^2 + \frac{1}{5} = 1 \Rightarrow A^2 = \frac{1}{2} - \frac{1}{5} = \frac{3}{10} \Rightarrow A = \sqrt{\frac{3}{10}}$$

Therefore, $|\psi(x,0)\rangle = \frac{1}{\sqrt{2}}|\phi_1\rangle + \sqrt{\frac{3}{10}}|\phi_1\rangle + \frac{1}{\sqrt{5}}|\phi_3\rangle$

Probabilities regarding the system to be in $|\phi_1\rangle, |\phi_2\rangle, |\phi_3\rangle$ states are

$$P_1 = |C_1|^2 = \frac{1}{2}, \quad P_2 = |C_2|^2 = \frac{3}{10}, \quad P_3 = |C_3|^2 = \frac{1}{5}$$

The state of the system at any time 't' will be

$$|\psi(x,t)\rangle = \frac{1}{\sqrt{2}}e^{-iE_1t/\hbar}|\phi_1\rangle + \sqrt{\frac{3}{10}}e^{-iE_2t/\hbar}|\phi_2\rangle + \frac{1}{\sqrt{5}}e^{-iE_3t/\hbar}$$

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Example 32: The wavefunction of a particle is given by $|\psi\rangle = \frac{1}{\sqrt{2}}|\phi_0\rangle + |\phi_1\rangle$ where $|\phi_0\rangle$ and $|\phi_1\rangle$ are the normalized eigenstates with energies E_0 and E_1 respectively. The hamiltonian in the state ψ is

(a) $\frac{E_0}{2} + E_1$ (b) $\frac{E_0}{2} - E_1$ (c) $\frac{E_0 - 2E_1}{3}$ (d) $\frac{E_0 + 2E_1}{3}$

Soln. Suppose normalized wavefunction: $|\psi\rangle = C\left[\frac{1}{\sqrt{2}}|\phi_0\rangle + |\phi_1\rangle\right]$ (where C is normalization constnat)

Normalization condition: $\langle\psi|\psi\rangle = 1 \quad \Rightarrow \quad \frac{C^3}{2} + C^2 = 1 \quad \Rightarrow C = \sqrt{\frac{2}{3}}$

Therefore, the normalized wavefunction will be

$$|\psi\rangle = \frac{1}{\sqrt{2}}|\phi_0\rangle + \sqrt{\frac{2}{3}}|\phi_2\rangle$$

Energy of the particle in the given state will be

$$\langle E\rangle = P(\phi_0)E_0 + P(\phi_1)E_1 = \frac{E_0 + 2E_1}{3}$$

2.6 Various Representation of wave function:

Wave function in position space is represented by $\psi(x)$

Wave function in momentum space or k-space is $\phi(p) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\psi(x)e^{-i\frac{p}{\hbar}x}dx$

Inverse relation: $\psi(x) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\phi(p)e^{i\frac{p}{\hbar}x}dp$

If a wave function is normalized in position space, it will be normalized in momentum space. But the normalization constant may be different.

Example 33. Find the wave function in k space for the wave packet

$$\psi_0(x) = Ae^{ik_0x} \qquad |x| \le a$$
$$= 0 \qquad |x| \ge a$$

Soln. Normalization condition:

$$\int_{-\infty}^{\infty}|\psi(x)|^2dx = 1 \Rightarrow A^2\int_{-a}^{a}dx = 1 \Rightarrow A^2\,2a = 1 \Rightarrow A = \frac{1}{\sqrt{2a}}$$

Therefore, $\psi_0(x) = \frac{1}{\sqrt{2a}}e^{ik_0x}$

So, the wave function in k-space will be

$$\phi(k) = \frac{1}{\sqrt{2a}}\frac{1}{\sqrt{2\pi}}\int_{-a}^{a}e^{ik_0x}e^{-ikx}dx = \frac{1}{2\sqrt{\pi a}}\int_{-a}^{a}e^{-i(k_0-k)x}dx$$

$$= \frac{1}{2\sqrt{\pi a}}\left[\frac{e^{i(k_0-k)x}}{i(k_0-k)}\right]_{-a}^{a} = \frac{1}{2\sqrt{\pi a}}\frac{2i\sin(k_0-k)a}{i(k_0-k)} = \frac{1}{\sqrt{\pi a}}\frac{\sin(k_0-k)a}{(k_0-k)}$$

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Example 34. Find the momentum representation $\phi(p)$ for the plane wave $\psi(x) = Ae^{\frac{ip_0}{\hbar}x}$

Soln. $\phi(p) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}Ae^{\frac{i(p_0-p)x}{\hbar}}dx$

$$= \frac{1}{\sqrt{2\pi\hbar}}A.2\pi.\delta\left(\frac{p_0-p}{\hbar}\right) = \sqrt{\frac{2\pi}{\hbar}}A\hbar\delta(p_0-p)$$

Therefore, the momentum space wave function will be $\phi(p) = A\sqrt{2\pi\hbar}\;\delta(p_0-p)$

Example 35. Find the momentum space wave function corresponding to the position space wave function of a particle at a given instant $\psi(x) = A\cos kx$

Soln. $\phi(p) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}A\cos kx\, e^{-i\frac{p}{\hbar}x}dx$

$$= \frac{A}{2\sqrt{2\pi\hbar}}\left[\int_{-\infty}^{\infty} e^{ix\left(k-\frac{p}{\hbar}\right)}dx + \int_{-\infty}^{\infty} e^{-ix\left(k+\frac{p}{\hbar}\right)}dx\right] = \frac{A}{2\sqrt{2\pi\hbar}}2\pi\hbar\left[\delta(\hbar k - p) + \delta(\hbar k + p)\right]$$

$$= \frac{A}{2}\sqrt{2\pi\hbar}\left[\delta(\hbar k - p) + \delta(\hbar k + p)\right]$$

• Probability Current density:

As the time changes from t = 0, the probability of finding the particle in some region of space may increase or decrease. If the probability increases in some region, then it should decrease in some other region such that total probability of finding the particle in the entire space should be equal to one. We can assume this as a flow of probability from one region to another region, like a fluid or current. Therefore, the probability flow satisfies the equation of continuity i.e.

$$\vec{\nabla}.\vec{J} + \frac{\partial \rho}{\partial t} = 0$$

where ρ = probability density $= \psi^* \psi$

and $\vec{J}$ = probability current density $= -\frac{i\hbar}{2m}\left[\psi^* \vec{\nabla}\psi - \psi \vec{\nabla}\psi^*\right]$

The magnitude of probability current density represents the flux of the particles i.e number of particles passing through per unit area per unit time and the direction of probability current density is along the direction of flow of the particles.

Example 36. A particle of mass 'm' is represented by wave function $\psi(x) = Ae^{ikx}$ (k = wave number, A = constant). The magnitude of probability current density is

(a) $|A|^2 \frac{\hbar k}{m}$ (b) $|A|^2 \frac{\hbar k}{2m}$ (c) $|A|^2 \frac{(\hbar k)^2}{m}$ (d) $|A|^2 \frac{(\hbar k)^2}{2m}$

Soln. Probability current density $=$

$$\vec{J} = -\frac{i\hbar}{2m}\left[\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x}\right]\hat{x} = \frac{i\hbar}{2m}\left[A^2 ik + A^2 ik\right]\hat{x} = |A|^2 \frac{\hbar k}{m}\hat{x}$$

Correct answer is (a)

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Example 37. The wave function of particle moving in free space is $\psi = e^{ikx} + 2e^{-ikx}$

(A) The probability current density for the real part of the wave function

(a) 1 (b) $\frac{\hbar k}{m}$ (c) $\frac{\hbar k}{2m}$ (d) 0

(B) The energy of the particle is

(a) $\frac{5\hbar^2 k^2}{2m}$ (b) $\frac{3\hbar^2 k^2}{2m}$ (c) $\frac{\hbar^2 k^2}{2m}$ (d) $\frac{\hbar^2 k^2}{m}$

Soln. **(A)** The real part of the wave function $\psi = e^{ikx} + 2e^{-ikx}$ is $3\cos kx$

Therefore, the corresponding probability density will be zero.

Correct answer is (d)

(B) $\hat{H}\psi = \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right)\psi = -\frac{\hbar^2}{2m}\left[\frac{d}{dx}\left\{ik\, e^{+ikx} - 2ik\, e^{-ikx}\right\}\right]$

$$= -\frac{\hbar^2}{2m}\left[-k^2 e^{ikx} - 2k^2 e^{-ikx}\right] = \frac{\hbar^2 k^2}{2m}\psi$$

Correct answer is (c)

Example 38. Calculate the probability current density for a Gaussian wave pocket

$$\psi(x) = A\exp\left[-\frac{x^2}{a^2} + \frac{ip_0 x}{\hbar}\right]$$

Soln. $$\vec{J} = -\frac{i\hbar}{2m}\left[\psi^* \frac{\partial\psi}{\partial x} - \psi\frac{\partial\psi^*}{\partial x}\right]\hat{x}$$

$$= -\frac{i\hbar}{2m}\left[A^* \exp\left(-\frac{x^2}{a^2} - i\frac{p_0 x}{\hbar}\right)\left(-\frac{2x}{a^2} + \frac{ip_0}{\hbar}\right) A\exp\left(-\frac{x^2}{a^2} + i\frac{p_0 x}{\hbar}\right)\right.$$

$$\left. - A\exp\left(-\frac{x^2}{a^2} + i\frac{p_0 x}{\hbar}\right)\left(-\frac{2x}{a^2} - \frac{ip_0}{\hbar}\right) A^* \exp\left(-\frac{x^2}{a^2} - i\frac{p_0 x}{\hbar}\right)\right]\hat{x}$$

$$= -\frac{i\hbar}{2m}\left[|A|^2 \exp\left(-\frac{2x^2}{a^2}\right)\left\{-\frac{2x}{a^2} + \frac{ip_0}{\hbar} + \frac{2x}{a^2} + \frac{ip_0}{\hbar}\right\}\right]\hat{x}$$

$$= \left(-\frac{i\hbar}{2m}\right)\left(\frac{2ip_0}{\hbar}\right)|A|^2 \exp\left(-\frac{2x^2}{a^2}\right)\hat{x} = \frac{p_0}{m}|A|^2 \exp\left(-\frac{2x^2}{a^2}\right)\hat{x}$$

Example 39. Calculate the probability current density for a 3-D wave function $\psi(r) = \frac{A}{r}e^{ikr}$

Soln. $$\vec{J} = -\frac{i\hbar}{2m}\left[\psi^* \frac{\partial\psi}{\partial r} - \psi\frac{\partial\psi^*}{\partial r}\right]\hat{r}$$

$$\vec{J} = -\frac{i\hbar}{2m}\left[\frac{A}{r}e^{-ikr}\left\{\frac{ik}{r}e^{ikr} - \frac{e^{ikr}}{r^2}\right\} - \frac{A}{r}e^{ikr}\left\{-\frac{ik}{r}e^{-ikr} - \frac{1}{r^2}e^{-ikr}\right\}\right]\hat{r}$$

$$= -\frac{i\hbar}{2m}\left[\frac{A^2}{r^2}\left(ik - \frac{1}{r} + ik + \frac{1}{r}\right)\right] = \frac{i\hbar}{2m}\frac{A^2}{r^2}2ik = \frac{\hbar k}{m}\frac{|A|^2}{r^2}$$

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Example 40. Show that for any normalized wave packet in one dimesion $\int_{-\infty}^{\infty} J(x)dx = \langle p_x\rangle/m$.

Soln. $$\int_{-\infty}^{\infty} J(x)dx = \frac{\hbar}{2im}\left[\int_{-\infty}^{\infty}\psi^*\frac{\partial}{\partial x}\psi dx - \int_{-\infty}^{\infty}\psi\frac{\partial}{\partial x}\psi^* dx\right]$$

$$= \frac{\hbar}{2im}\left[\frac{1}{-i\hbar}\int_{-\infty}^{\infty}\psi^* dx\left(-i\hbar\frac{d}{dx}\right)\psi(x) - c.c.\right]$$

where c.c. is the complex conjugate of the first term. Now, $\langle p_x\rangle$ must be real. So, the first term in the square bracket is $\frac{1}{-i\hbar}\langle p_x\rangle$ and hence its complex conjugate is $\frac{1}{i\hbar}\langle p_x\rangle$.

Thus, $\int_{-\infty}^{\infty} J(x)\,dx = \frac{\hbar}{2im}\left[\frac{2}{-i\hbar}\langle p_x\rangle\right] = \frac{\langle p_x\rangle}{m}$

Example 41. The solution of the Schrodinger equation for a free particle of mass m in one dimension i $\psi(x,t)$. At $t=0$, $\psi(x,0) = A\exp\left(\frac{-x^2}{a^2}\right)$. Find the probability amplitude in momentum space at $t=0$ an at time t.

Soln. $\Phi(p,0) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\psi(x,0)\exp\left(-\frac{ipx}{\hbar}\right)dx$

$= \frac{A}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\exp\left(-\frac{x^2}{a^2}-\frac{ipx}{\hbar}\right)dx = \frac{Aa}{\sqrt{2\hbar}}\exp\left(-\frac{p^2a^2}{4\hbar^2}\right)$

The Schrodinger equation for the momentum space equation is

$i\hbar\frac{\partial\Phi}{\partial t} = \frac{p^2}{2m}\Phi \Rightarrow \frac{d\Phi}{\Phi} = \left(\frac{ip^2}{2m\hbar}\right)dt \Rightarrow \Phi(p,t) = C\exp\left(\frac{ip^2t}{2m\hbar}\right)$

At $t=0, \Phi(p,0) = C$ Hence,

$\Phi(p,t) = \frac{Aa}{\sqrt{2\hbar}}\exp\left(-\frac{p^2a^2}{4\hbar^2}-\frac{ip^2t}{2m\hbar}\right)$

CSIR-NET PREVIOUS YEAR SOLVED QUESTIONS

Q.1. The commutator $\left[x^2, p^2\right]$ is: **[CSIR June 2012]**

(a) $2i\hbar\,xp$ (b) $2i\hbar(xp+px)$ (c) $2i\hbar px$ (d) $2i\hbar(xp-px)$

Soln. $\left[x^2,p^2\right] = x\left[x,p^2\right]+\left[x,p^2\right]x$ (Using the property $[AB,C] = A[B,C]+[A,C]B$)

$= 2i\hbar\,xp + 2i\hbar\,px = 2i\hbar(xp+px)$ (Using the property: $\left[A,B^n\right] = nB^{n-1}[A,B]$)

Correct Option is (b).

Q.2. Which of the following is a self-adjoint operator in the spherical polar coordinate system (r,θ,φ)? **[CSIR June 2012]**

(a) $-\frac{i\hbar}{\sin^2\theta}\frac{\partial}{\partial\theta}$ (b) $-i\hbar\frac{\partial}{\partial\theta}$ (c) $-\frac{i\hbar}{\sin\theta}\frac{\partial}{\partial\theta}$ (d) $-i\hbar\sin\theta\frac{\partial}{\partial\theta}$

Soln. An operator is said to be self-adjoint if $\int\phi^*\hat{A}\,\psi\,d\tau = \int\left(\hat{A}\phi\right)^*\psi\,d\tau$

$\int_{r=0}^{\infty}\int_{\theta=0}^{\pi}\int_{\varphi=0}^{2\pi}\phi^*(r,\theta,\varphi)\left(\frac{-i\hbar}{\sin\theta}\frac{\partial}{\partial\theta}\right)\psi(r,\theta,\varphi)\,r^2dr\,\sin\theta\,d\theta\,d\varphi$

$= -i\hbar\int_{r=0}^{\infty}\int_{\theta=0}^{\pi}\int_{\varphi=0}^{2\pi}\phi^*(r,\theta,\varphi)\frac{\partial\psi}{\partial\theta}(r,\theta,\varphi)\,r^2drd\theta\,d\varphi$

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Q.3.

Soln.

Q.4.

On integrating by parts w.r.t θ we get, $= \int_{r=0}^{\infty}\int_{\theta=0}^{\pi}\int_{\varphi=0}^{2\pi}\left(\frac{-i\hbar}{\sin\theta}\frac{\partial\phi}{\partial\theta}\right)^{*}\psi\, r^2\sin\theta\, dr\, d\theta\, d\varphi$

ension i

$t=0$ and

$$=\int_{r=0}^{\infty}\int_{\theta=0}^{\pi}\int_{\varphi=0}^{2\pi}\left(\frac{i\hbar}{\sin\theta}\frac{\partial\phi^{*}}{\partial\theta}\right)\psi\, r^2\sin\theta dr\, d\theta\, d\varphi=\int_{r=0}^{\infty}\int_{\theta=0}^{\pi}\int_{\varphi=0}^{2\pi}\left(\frac{-i\hbar}{\sin\theta}\frac{\partial\phi}{\partial\theta}\right)^{*}\psi\, r^2\sin\theta dr\, d\theta\, d\varphi$$

So, $\left(\frac{-i\hbar}{\sin\theta}\frac{\partial}{\partial\theta}\right)^{\dagger}=\frac{-i\hbar}{\sin\theta}\frac{\partial}{\partial\theta}$

Correct answer is (c).

Q.3. Given the usual canonical commutation relations, the commutator $[A,B]$ of $A=i\left(xp_y-yp_x\right)$ and $B=\left(yp_z+zp_y\right)$ is : **[CSIR Dec 2012]**

(a) $\hbar\left(xp_z-p_xz\right)$ (b) $-\hbar\left(xp_z-p_xz\right)$ (c) $\hbar\left(xp_z+p_xz\right)$ (d) $-\hbar\left(xp_z+p_xz\right)$

Soln. $A=i\left(xp_y-yp_x\right)$ & $B=\left(yp_z+zp_y\right)$

$$[A,B]=\left[i\left(xp_y-yp_x\right),\left(yp_z+zp_y\right)\right]$$

$$=i\left[xp_y,yp_z\right]-i\left[yp_x,yp_z\right]+i\left[xp_y,zp_y\right]-i\left[yp_x,zp_y\right]$$

[Out of 4 commutation relations 2nd and 3rd will be zero as there will be no canonically conjugate pair term]

So, $[A,B]=i\left[xp_y,yp_z\right]-i\left[yp_x,zp_y\right]$

$$=ix\left[p_y,yp_z\right]+i\left[x,yp_z\right]p_y-iy\left[p_x,zp_y\right]-i\left[y,zp_y\right]p_x$$

[Out of 4 commutation relations 2nd and 3rd will be zero as there will be no canonically conjugate pair term]

So, $[A,B]=ix\left[p_y,yp_z\right]-i\left[y,zp_y\right]p_x$

$$=ixy\left[p_y,p_z\right]+ix\left[p_y,y\right]p_z-iz\left[y,p_y\right]p_x-i\left[y,z\right]p_yp_x$$

Therefore, $[A,B]=0+ix\left(-i\hbar\right)p_z-iz\left(i\hbar\right)p_x-0$

$$=\hbar\left(xp_z+zp_x\right)=\hbar\left(xp_z+p_xz\right)$$

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Correct option is (c)

Q.4. If a particle is represented by the normalized wave function

$$\psi(x)=\begin{cases}\dfrac{\sqrt{15}\left(a^2-x^2\right)}{4a^{5/2}} & \text{for } -a<x<a\\ 0 & \text{otherwise}\end{cases}$$

the uncertainty Δp in its momentum is **[CSIR Dec 2012]**

(a) $\frac{2\hbar}{5a}$ (b) $\frac{5\hbar}{2a}$ (c) $\frac{\sqrt{10}\,\hbar}{a}$ (d) $\frac{\sqrt{5}\,\hbar}{\sqrt{2}\,a}$

Soln. $\langle p\rangle = \int_{-\infty}^{\infty} \psi^*\left(-i\hbar\frac{d}{dx}\right)\psi dx = \int_{-a}^{+a} \frac{\sqrt{15}}{4a^{5/2}}\left(a^2-x^2\right)\left(-i\hbar\frac{d}{dx}\right)\frac{\sqrt{15}}{4a^{5/2}}\left(a^2-x^2\right)dx$

$= -i\hbar\int_{-a}^{+a}\frac{15}{16a^5}\left(a^2-x^2\right)(-2x)\,dx = 0$ [As the function given in the integral is odd]

On the other hand, the expectation value of momentum for a real wavefunction is always zero.

$$\langle p^2\rangle = \int_{-\infty}^{+\infty}\psi^*\left(-\hbar^2\frac{d^2}{dx^2}\right)\psi dx = \frac{15}{16a^5}\int_{=a}^{a}\left(a^2-x^2\right)\left(-\hbar^2\frac{d^2}{dx^2}\right)\left(a^2-x^2\right)dx$$

$$= -\hbar^2\int_{-a}^{+a}\frac{15}{16\,a^5}\left(a^2-x^2\right)(-2)\,dx = \frac{5}{2}\frac{\hbar^2}{a^2}$$

Uncertainity in momentum $\Delta p = \sqrt{\langle p^2\rangle - \langle p\rangle^2} = \sqrt{\frac{5}{2}\left(\frac{\hbar}{a}\right)^2} = \frac{\sqrt{5}}{\sqrt{2}}\frac{\hbar}{a}$

Correct option is (d)

Q.5. If the operators A and B satisfy the commutation relation [A, B] = I, where I is the identity operator, then **[CSIR June 2013]**

(a) $[e^A, B] = e^A$ (b) $[e^A, B] = [e^B, A]$

(c) $[e^A, B] = [e^{-B}, A]$ (d) $[e^A, B] = 1$

Soln. $[A,B] = I \quad \& \quad e^A = 1 + A + \frac{A^2}{2!} + \frac{A^3}{3!} + \ldots\ldots$

$$\left[e^A, B\right] = \left[1 + A + \frac{A^2}{2!} + \frac{A^3}{3!} + \ldots\ldots, B\right]$$

$$= [1,B] + [A,B] + \frac{1}{2!}\left[A^2, B\right] + \frac{1}{3!}\left[A^3, B\right] + \ldots\ldots$$

$$= 0 + I + \frac{1}{2!}(2A)[A,B] + \frac{1}{3!}\left(3A^2\right)[A,B] + \ldots\ldots$$

$$= I + A + \frac{A^2}{2!} + \ldots\ldots = e^A$$

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Correct answer is (a)

Q.6. If A, B and C are non-zero Hermitian operators, which of the following relations must be false? **[CSIR Dec 2013]**

(a) [A, B] = C (b) AB + BA = C (c) ABA = C (d) A+ B = C

Soln. Given : $A^\dagger = A, B^\dagger = B, C^\dagger = C$

$$C = [A,B] = AB - BA \Rightarrow C^\dagger = (AB-BA)^\dagger = B^\dagger A^\dagger - A^\dagger B^\dagger = BA - AB = -C$$

So, C = [A, B] is not hermitian.

Correct answer is (a)

Conc

Q.7.

Soln.

Q.8.

Soln.

Q.7. Let x and p denote, respectively, the coordinate and momentum operators satisfying the canonical commutation relation $[x, p] = i$ in natural units ($\hbar = 1$). Then the commutator $[x, pe^{-p}]$ is **[CSIR Dec 2014]**

(a) $i(1-p)e^{-p}$ (b) $i(1-p^2)e^{-p}$ (c) $i(1-e^{-p})$ (d) ipe^{-p}

Soln. $\left[x, pe^{-p}\right] = [x,p]e^{-p} + p\left[x, e^{-p}\right]$ (Using the property $[A,BC] = [A,B]C + B[A,C]$)

$$= ie^{-p} + p\left[x, \left(1 - p + \frac{p^2}{2!} - \frac{p^3}{3!} + \ldots\ldots\right)\right]$$

$$= ie^{-p} + p\left([x,1] - [x,p] + \frac{1}{2!}\left[x, p^2\right] - \frac{1}{3!}\left[x, p^3\right] + \ldots\ldots\right)$$

$$= ie^{-p} + p\left(0 - i + \frac{1}{2!}2p[x,p] - \frac{1}{3!}3p^2[x,p] + \ldots\ldots\right)$$

$$= ie^{-p} + p\left(-i + ip - i\frac{p^2}{2!} + \ldots\ldots\right) = ie^{-p} - ip\left(1 - p + \frac{p^2}{2!} - \frac{p^3}{3!} + \ldots\ldots\right)$$

Correct Option is (a)

Q.8. Suppose the Hamiltonian of a conservative system in classical mechanics is $H = \omega xp$, where ω is a constant and x and p are the position and momentum respectively. The corresponding Hamiltonian in quantum mechanics, in the coordinate representation, is **[CSIR Dec 2014]**

(a) $-i\hbar\omega\left(x\frac{\partial}{\partial x} - \frac{1}{2}\right)$ (b) $-i\hbar\omega\left(x\frac{\partial}{\partial x} + \frac{1}{2}\right)$ (c) $-i\hbar\omega x\frac{\partial}{\partial x}$ (d) $-\frac{i\hbar\omega}{2}x\frac{\partial}{\partial x}$

Soln. Given: Hamiltonian of a conservative system in classical mechanics is $H = \omega xp$

In Quantum mechanics, the position and momentum operator does not commute i.e. $[x, p] = i\hbar$

Therefore, the corresponding Hamiltonian in Quantum mechanics can be written as

$$H = \omega\left(\frac{xp + px}{2}\right) = \omega\left(\frac{xp + xp - i\hbar}{2}\right) = \omega\left(xp - \frac{i\hbar}{2}\right)$$

$$\Rightarrow H = \omega\left[x\left(-i\hbar\frac{\partial}{\partial x}\right) - \frac{i\hbar}{2}\right] = -i\hbar\omega\left[x\frac{\partial}{\partial x} + \frac{1}{2}\right]$$

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Correct Option is (b)

PRACTICE SET

1. $\hat{A}$ and $\hat{B}$ are two quantum mechanical operators. If $\left[\hat{A},\hat{B}\right]$ stands for the commutator of $\hat{A}$ and $\hat{B}$, the $\left[\left[\hat{A},\hat{B}\right],\left[\hat{B},\hat{A}\right]\right]$ is equal to **[GATE 2002]**

(a) $\hat{A}\hat{B}\hat{A}\hat{B}-\hat{B}\hat{A}\hat{B}\hat{A}$ (b) $\hat{A}\left(\hat{A}\hat{B}-\hat{B}\hat{A}\right)-\hat{B}\left(\hat{B}\hat{A}-\hat{A}\hat{B}\right)$ (c) zero (d) $\left(\left[\hat{A},\hat{B}\right]\right)^2$

2. The commutator $\left[x,P^2\right]$, where x and P are position and momentum operators respectively, is **[GATE 2003]**

(a) $2i\hbar P$ (b) $-i\hbar P$ (c) $2i\,\hbar\,x\,P$ (d) $-2i\,\hbar\,x\,P$

3. If $\left[x,p\right]=i\hbar$, the value of $\left[x^3,p\right]$ is **[GATE 2007]**

(a) $2i\hbar x^2$ (b) $-2i\hbar x^2$ (c) $3i\hbar x^2$ (d) $-3i\hbar x^2$

4. Three operators X,Y and Z satisfy the commutation relations

$\left[X,Y\right]=i\hbar Z,\left[Y,Z\right]=i\hbar X$ and $\left[Z,X\right]=i\hbar Y$

The set of all possible eigenvalues of the operator Z, in units of $\hbar$, is **[GATE 2007]**

(a) $\{0,\pm1,\pm2,\pm3,.....\}$ (b) $\left\{\frac{1}{2},1,\frac{3}{2},2,\frac{5}{2},.....\right\}$

(c) $\left\{0,\pm\frac{1}{2},\pm1,\pm\frac{3}{2},\pm2,\pm\frac{5}{2},.....\right\}$ (d) $\left\{-\frac{1}{2},+\frac{1}{2}\right\}$

5. $\hat{A}$ and $\hat{B}$ represents two physical characteristics of a quantum system. If $\hat{A}$ is Hermitian, then for the produc $\hat{A}\hat{B}$ to be Hermitian, it is sufficient that **[GATE 2009]**

(a) $\hat{B}$ is Hermitian (b) $\hat{B}$ is anti-Hermitian

(c) $\hat{B}$ is Hermitian and $\hat{A}$ and $\hat{B}$ commute (d) $\hat{B}$ is Hermitian and $\hat{A}$ and $\hat{B}$ is anti-commute.

6. Which one of the functions given beow represents the bound state eigen function of the operator $-\frac{d^2}{dx^2}$ in the region $0\le x<\infty$, with the eigenvalue -4? **[GATE 2009]**

(a) A_0e^{2x} (b) $A_0\cosh 2x$ (c) A_0e^{-2x} (d) $A_0\sinh 2x$

7. Consider a quantum mechanical system with three linear operators $\hat{A}$, $\hat{B}$ and $\hat{C}$, which are related b

$$\hat{A}\hat{B}-\hat{C}=\hat{I}$$

where $\hat{I}$ is the unit operator. If $\hat{A}=\frac{d}{dx}$ and $\hat{B}=x$, then $\hat{C}$ must be **[TIFR 2013]**

(a) zero (b) $\frac{d}{dx}$ (c) $-x\frac{d}{dx}$ (d) $x\frac{d}{dx}$

8. The state $|\psi\rangle$ of a quantum mechanical system, in a certain basis, is represented by the column vector

$$|\psi\rangle=\begin{pmatrix}1/\sqrt{2}\\0\\1/\sqrt{2}\end{pmatrix}$$

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The operator $\hat{A}$ corresponding to a dynamical variable A, is given, in the same basis, by the matrix

$$\hat{A}=\begin{pmatrix}1 & 1 & 1\\ 1 & 2 & 1\\ 1 & 1 & 2\end{pmatrix}.$$

If, now, a measurement of the variable A is made on the system in the state $|\psi\rangle$, the probability that the result will be +1 is **[TIFR 2013]**

(a) $\frac{1}{\sqrt{2}}$ (b) 1 (c) $\frac{1}{2}$ (d) $\frac{1}{4}$

9. The hermitian eonjugate of the operator $(-\partial/\partial x)$ is **[JEST 2013]**

(a) $\partial/\partial x$ (b) $-\partial/\partial x$ (c) $i\partial/\partial x$ (d) $-i\partial/\partial x$

10. The operator $\left(\frac{d}{dx}-x\right)\left(\frac{d}{dx}+x\right)$ is equivalent to **[JEST 2013]**

(a) $\frac{d^2}{dx^2}-x^2$ (b) $\frac{d^2}{dx^2}-x^2+1$

(c) $\frac{d^2}{dx^2}-x\frac{d}{dx}x^2+1$ (d) $\frac{d^2}{dx^2}-2x\frac{d}{dx}-x^2$

11. The operator A and B share all the eigenstates. Then the least possible value of the product of uncertainties $\Delta A\Delta B$ is **[JEST 2014]**

(a) $\hbar$ (b) 0 (c) $\hbar/2$ (d) Determinant (AB)

12. A normalized state of a particle moving in a potential $V(x)$ is given by

$$\psi(x,t)=\sum_{n=0}^{\infty}C_n\phi_n(x)e^{-E_nt/\hbar}$$

where $\phi_n(x)$'s are the normalized eigenfunctions of the particle corresponding to the energies E_n's. Then **[GATE 2001]**

(a) $\sum_{n=0}|C_n|^2=1$

(b) The average energy of the particle in the state $\psi(x,t)$ is $\sum_{n=\infty}^{\infty}|C_n|^2E_n$

(c) $\psi(x,t)$ is an eigenfunction of the Hamiltonian of the particle.

(d) $\psi(x,t)$ is an eigenfunction of the momentum operator.

13. Which of the following functions represents acceptable wave function of a particle in the range $-\infty\le x\le\infty$. **[GATE 2001]**

(a) $\varphi(x)=A\tan x, A>0$ (b) $\varphi(x)=B\cos x, B$ real

(c) $\varphi(x)=C\exp(-D/x^2), C>0, D<0$ (d) $\varphi(x)=E\,x\exp(-Fx^2), E,F>0$

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14. An electron in a time independent potential is in a state which is a superposition of the ground state ($E_0 = 11\,eV$) and the first excited state ($E_1 = 1\,eV$). The wave function of the electron will repeat itself with a period of **[GATE 2003]**

(a) 3.1×10^{-18} sec (b) 2.1×10^{-15} sec (c) 1.2×10^{-12} sec (d) 1.0×10^{-9} sec

16. A particle has the wave function $\psi(x,t) = A\left[\exp(i\omega t)\cos(kx)\right]$. Which one of the following is correct? **[GATE 2003]**

(a) This is an eigen state of both energy and momentum.

(b) This is an eigen state of momentum and not energy.

(c) This is an eigen state of energy and not momentum.

(d) This is not an eigen state of energy or momentum.

Commom data for Q. 17 and Q.18

The normalized wave function ψ_1 and ψ_2 correspond to the ground state and the first excited state of a particle in a potential. You are given the information that the operator $\hat{A}$ acts on the wave functions as $\hat{A}\psi_1 = \psi_2$ and $\hat{A}\psi_2 = \psi_1$ **[GATE 2003]**

17. The expectation value of A for the state $\psi = (3\psi_1 + 4\psi_2)/5$ is

(a) –0.32 (b) 0.0 (c) 0.75 (d) 0.96

18. Which of the following are eigenfunctions of $\hat{A}^2$?

(a) ψ_1 and ψ_2 (b) ψ_2 and not ψ_1 (c) ψ_1 and not ψ_2 (d) neither ψ_1 and ψ_2

19. The time independent Schrodinger equation of a system reprersents the conservation of the **[GATE 2004]**

(a) total binding energy of the system. (b) total potential energy of the system.

(c) total kinetic energy of the system. (d) total energy of the system.

20. A system in a normalized state $|\psi\rangle = c_1|\alpha_1\rangle + c_2|\alpha_2\rangle$, with $|\alpha_1\rangle$ and $|\alpha_2\rangle$ representing two different eigenstates of the system, requires that the constants c_1 and c_2 must satisfy the condition **[GATE 2005]**

(a) $|c_1|.|c_2| = 1$ (b) $|c_1| + |c_2| = 1$ (c) $(|c_1| + |c_2|)^2 = 1$ (d) $|c_1|^2 + |c_2|^2 = 1$

21. The parities of the wave functions (i) $\cos kx$ and (ii) $\tanh kx$ are **[GATE 2005]**

(a) odd, odd (b) even, even (c) odd, even (d) even, odd

22. If the probability that x lies between x and x+dx is $p(x)\,dx = ae^{-ax}$, where $0 < x < \infty$, $a > 0$, then the probability that x lies between x_1 and $x_2\,(x_2 > x_1)$ is: **[GATE 2005]**

(a) $\left(e^{-ax_1} - e^{-ax_2}\right)$ (b) $a\left(e^{-ax_1} - e^{-ax_2}\right)$ (c) $e^{-ax_2}\left(e^{-ax_1} - e^{-ax_2}\right)$ (d) $e^{-ax_1}\left(e^{-ax_1} - e^{-ax_2}\right)$

23. The wavefunction of a particle in a one-dimensional potential at time $t = 0$ is

$$\psi(x, t=0) = \frac{1}{\sqrt{15}}\left[2\psi_0(x) - \psi_1(x)\right]$$

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where $\psi_0(x)$ and $\psi_1(x)$ are the ground and the first excited states of the particle with corresponding energies E_0 and E_1. The wavefunction of the particle at a time 't' is: **[GATE 2006]**

(a) $\frac{1}{\sqrt{5}} e^{i(E_0+E_1)t/2\hbar}\left[2\psi_0(x)-\psi_1(x)\right]$ (b) $\frac{1}{\sqrt{5}} e^{-iE_0t/\hbar}\left[2\psi_0(x)-\psi_1(x)\right]$

(c) $\frac{1}{\sqrt{5}} e^{-iE_0t/\hbar}\left[2\psi_0(x)-\psi_1(x)\right]$ (d) $\frac{1}{\sqrt{15}}\left[2\psi_0(x)e^{-iE_0t/\hbar}-\psi_1(x)e^{-iE_1t/\hbar}\right]$

24. A particle of mass m is represented by the wavefunction $\psi(x) = Ae^{ikx}$, where k is the wavevector and A is a constant. The magnitude of the probability current density of the particle is **[GATE 2006]**

(a) $|A|^2\frac{\hbar k}{m}$ (b) $|A|^2\frac{\hbar k}{2m}$ (c) $|A|^2\frac{(\hbar k)^2}{m}$ (d) $|A|^2\frac{(\hbar k)^2}{2m}$

25. The wave function of a particle, moving in a one-dimensional time-independent potential V(x), is given by $\psi(x) = e^{-iax+b}$, where a and b are constants. This means that the potential $V(x)$ is of the form **[GATE 2007]**

(a) $V(x) \propto x$ (b) $V(x) \propto x^2$ (c) $V(x) = 0$ (d) $V(x) \propto e^{-ax}$

26. A particle is in the normalized state $|\psi\rangle$ which is superposition of the energy eigenstates $|E_0 = 10\text{ eV}\rangle$ and $|E_1 = 30\text{ eV}\rangle$. The average value of energy of the particle in the state $|\psi\rangle$ is 20 eV. The state $|\psi\rangle$ is given by **[GATE 2009]**

(a) $\frac{1}{2}|E_0 = 10\text{ eV}\rangle + \frac{\sqrt{3}}{4}|E_1 = 30\text{ eV}\rangle$ (b) $\frac{1}{\sqrt{3}}|E_0 = 10\text{ eV}\rangle + \sqrt{\frac{2}{3}}|E_1 = 30\text{ eV}\rangle$

(c) $\frac{1}{2}|E_0 = 10\text{ eV}\rangle + \frac{\sqrt{3}}{4}|E_1 = 30\text{ eV}\rangle$ (d) $\frac{1}{\sqrt{2}}|E_0 = 10\text{ eV}\rangle - \frac{1}{\sqrt{2}}|E_1 = 30\text{ eV}\rangle$

27. Which of the following is an allowed wavefunction for a particle in a bound state? N is a constant and $\alpha, \beta > 0$. **[GATE 2009]**

(a) $\psi = N\frac{e^{-\alpha r}}{r^3}$ (b) $\psi = N(1-e^{-\alpha r})$

(c) $\psi = Ne^{-\alpha x}e^{-\beta(x^2+y^2+z^2)}$ (d) $\psi = \begin{cases} \text{non-zero constant} & \text{if } r < R \\ 0 & \text{if } r > R \end{cases}$

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Common data for Q. 28 and Q. 29

The wavefunction of a particle moving in free space is given by, $\psi = e^{ikx} + 2e^{-ikx}$

28. The energy of the particle is **[GATE 2012]**

(a) $\frac{5\hbar^2k^2}{2m}$ (b) $\frac{3\hbar^2k^2}{4m}$ (c) $\frac{\hbar^2k^2}{2m}$ (d) $\frac{\hbar^2k^2}{m}$

29. The probability current density for the real part of the wavefunction is

(a) 1 (b) $\frac{\hbar k}{m}$ (c) $\frac{\hbar k}{2m}$ (d) 0

30. Consider the wave function $Ae^{ikr}(r_0/r)$, where A is the normalization constant. For $r = 2r_0$, the magnitude of probability current density up to two decimal places, in units of $(A^2\hbar k/m)$, is _____.

[GATE 2013]

31. In a quantum mechanical system, an observable A is represented by an operator $\hat{A}$. If $|\psi\rangle$ is a state of the system, but not an eigenstate of $\hat{A}$, then the quantity

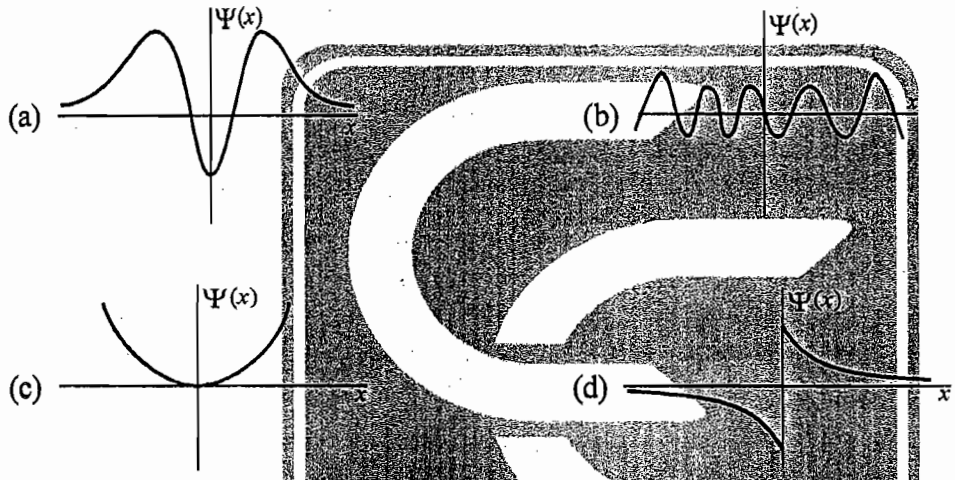
$$r = \langle\psi|\hat{A}|\psi\rangle^2 - \langle\psi|\hat{A}^2|\psi\rangle$$

satisfies the relation **[TIFR 2013]**

(a) $r < 0$ (b) $r = 0$ (c) $r > 0$ (d) $r \geq 0$

32. A particle of energy E moves in one dimension under the influence of a potentials $V(x)$. If $E > V(x)$ for some range of x, which of the following graphs can represent a bound state wave function of the particle?

[TIFR 2013]



33. A particle moving in a one dimension has the un-normalised wave function

$$\psi(x) = x\exp\left(-\frac{x^2}{\lambda^2}\right)$$

where λ is a real constant. The expectation value of its momentum is **[TIFR 2014]**

(a) $\frac{\hbar}{\lambda}\exp\left(-\frac{x^2}{\lambda^2}\right)$ (b) $\frac{\hbar}{\lambda^2} - 2\frac{\hbar}{\lambda}$ (c) $\frac{\hbar}{\lambda}\exp(-1)$ (d) zero

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34. A two state quantum system has two observables A and B. It is known that the observable A has eigenstates $|\alpha_1\rangle$ and $|\alpha_2\rangle$ with eigenvalues a_1 and a_2 respectively, while B has eigenstates $|\beta_1\rangle$ and $|\beta_2\rangle$ with eigenvalues b_1 and b_2 respectively, and that these eigenstates are related by

[TIFR 2015]

$$|\beta_1\rangle = \frac{3}{5}|\alpha_1\rangle - \frac{4}{5}|\alpha_2\rangle \qquad |\beta_2\rangle = \frac{4}{5}|\alpha_1\rangle + \frac{3}{5}|\alpha_2\rangle$$

Suppose a measurement is made of the observable A and a value a_1 is obtained. If the observable B is now measured, the probability of obtaining the value b_1 will be

(a) 0.80 (b) 0.64 (c) 0.60 (d) 0.36

35. The wave function of a free particle in one dimension is given by $\psi(x) = A\sin x + B\sin 3x$. Then $\psi(x)$ is an eigenstate of **[JEST 2012]**

(a) the position operator
(b) the Hamiltonian
(c) the momentum operator
(d) the parity operator

36. The quantum state $\sin x|\uparrow\rangle + \exp(i\phi)\cos x|\downarrow\rangle$, where $\langle\uparrow||\downarrow\rangle = 0$ and x, ϕ are, real, is orthogonal to: **[JEST 2012]**

(a) $\sin x|\uparrow\rangle$ (b) $\cos x|\uparrow\rangle + \exp(i\phi)\sin x|\downarrow\rangle$

(c) $-\cos x|\uparrow\rangle - \exp(i\phi)\sin x|\downarrow\rangle$ (d) $-\exp(i\phi)\cos x|\uparrow\rangle + \sin x|\downarrow\rangle$

37. If the expectation value of the momentum is $\langle p\rangle$ for the wavefunction $\psi(x)$, then the expectation value of momentum for the wavefunction $e^{ikx/\hbar}\psi(x)$ is **[JEST 2013]**

(a) k (b) $\langle p\rangle - k$ (c) $\langle p\rangle + k$ (d) $\langle p\rangle$

38. The Hamiltonian operator for a two-state system is given by

$$H = a\left(|1\rangle\langle 1| - |2\rangle\langle 2| + |1\rangle\langle 2| + |2\rangle\langle 1|\right)$$

where 'a' is a positive number with the dimension of energy. The energy eigenstates corresponding to the larger and smaller eigenvalues respectively are **[JEST 2014]**

(a) $|1\rangle - (\sqrt{2}+1)|2\rangle, |1\rangle + (\sqrt{2}-1)|2\rangle$ (b) $|1\rangle + (\sqrt{2}-1)|2\rangle, |1\rangle - (\sqrt{2}+1)|2\rangle$

(c) $|1\rangle + (\sqrt{2}-1)|2\rangle, (\sqrt{2}+1)|1\rangle - |2\rangle$ (d) $|1\rangle - (\sqrt{2}-1)|2\rangle, (\sqrt{2}+1)|1\rangle + |2\rangle$

39. Consider a three-state system with energies E, E, and E−3g (where g is a constant) and respective eigenstates

$$|\psi_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\\0\end{pmatrix},\quad |\psi_2\rangle = \frac{1}{\sqrt{6}}\begin{pmatrix}1\\1\\-2\end{pmatrix},\quad |\psi_3\rangle = \frac{1}{\sqrt{3}}\begin{pmatrix}1\\1\\1\end{pmatrix}$$

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If the system is initially (at $t = 0$) in state

$$|\psi_i\rangle = \begin{pmatrix}1\\0\\0\end{pmatrix}$$

What is the probability that at a later time 't' system will be in state

$$|\psi_f\rangle = \begin{pmatrix}0\\0\\1\end{pmatrix}$$

[JEST 2014]

(a) 0 (b) $\frac{4}{9}\sin^3\left(\frac{3gt}{2\hbar}\right)$ (c) $\frac{4}{9}\cos^2\left(\frac{3gt}{2\hbar}\right)$ (d) $\frac{4}{9}\sin^2\left(\frac{E-3gt}{2\hbar}\right)$

40. A ball bounces back off earth. You are asked to solve this quantum mechanically assuming the earth is a infinitely hard sphere. Consider surface of earth as the origin implying $V(0) = \infty$ and a linear potential eleswher (i.e. $V(x) = -mgx \ for \ x > 0$). Which of the following wave function is physically admissible for this proble (with $k > 0$): **[JEST 2014]**

(a) $\psi(x) = \frac{e^{-kx}}{x}$ (b) $\psi(x) = xe^{-kx^2}$ (c) $\psi(x) = -Axe^{kx}$ (d) $\psi(x) = Axe^{-kx^2}$

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Chapter 3

One-dimensional potentials

3.1 Introduction to Bound States :

If the motion of a particle is confined to a limited region of space by potential energy so that the particle can move back and forth in the region, then the particle is in a bound state. The simplest example of all motions in bound state is the motion of a particle in a one-dimensional box with zero potential energy and the potential energy is assumed to be infinite at the walls of the box.

The motion of a particle in three-dimensional box, one-dimensional box, motion of a simple harmonic oscillator, motion of a particle in a one-dimensional square well potential with ($E < V_0$), motion of a particle in a one-dimensional square well potential with ($E < V_0$), motion of a particle in one-dimensional (also in three-dimensional) potential well, motion of a particle in spherically symmetric potential, etc. are the common examples of bound state. Application of Schrodinger time-independent equal to such problems leads to discrete energy values of the particles.

Properties of 1-D bound states:

(i) Energy eigenstates corresponding to one dimensional bounds states are of discrete energy and non-degenerate in nature.

(ii) The wavefunction of a particle moving under a one dimensional symmetric potential should have a definite parity i.e. it will be either even or odd parity.

(iii) The wavefunction of a particle in the n^{th} state will have n-nodes if n = 0 corresponds to the ground state of the particle and will have n-1 nodes if n = 1 corresponds to the ground state of the particles.

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3.2 One-dimensional infiitely deep potential well

Consider a particle of mass 'm' and energy 'E' is moving along x-axis, in the region from $x = 0$ to $x = a$ under the following potential i.e.

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$$V(x) = 0 \qquad 0 < x < a$$

$$= \infty \qquad \text{otherwise}$$

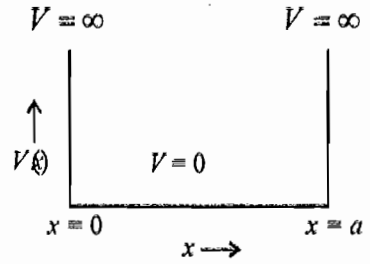

Figure : Schematic diagram of 1-D infinite potential well.

The particle experiences no force within the potential well but feels a sudden large force directed towards the origin as it reaches the points $x = 0, a$. Since, the potential is infinite outside, the particle cannot penetrate outside of the region $0 < x < a$ i.e. $\psi = 0$ for the particle outside the box.

According to 1-D time-independent Schrodinger equaion,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+V\psi(x)=E\psi(x) \tag{1}$$

For the region $0<x<a$, the equation becomes,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}=E\psi \qquad \Rightarrow \frac{d^2\psi}{dx^2}+\frac{2mE}{\hbar^2}\psi=0$$

$$\Rightarrow \frac{d^2\psi}{dx^2}+k^2x=0 \text{ where } k^2=\frac{2mE}{\hbar^2} \tag{2}$$

Solution of eqn. (2) can be written as,

$$\psi(x)=A\sin kx+B\cos kx \tag{3}$$

Since, the particle remains confined within the box, then the probablity of finding the particle at $x = 0$ and $x = a$ must be zero.

Boundary conditions: $\psi(x)$ will be continuous at $x = 0$ and $x = a$

(i) Applying $\psi(x)|_{x=0}=0 \Rightarrow B=0$

(ii) Applying $\psi(x)|_{x=a}=0 \Rightarrow A\sin ka=0 \Rightarrow ka=n\pi \Rightarrow k=\frac{n\pi}{a}$

$$\Rightarrow \psi(x)=A\sin\left(\frac{n\pi x}{a}\right)(n=1,2,3,.....) \text{ for } 0<x<a \tag{4}$$

Note: If $n=0 \Rightarrow k=0 \Rightarrow E=0 \Rightarrow \psi(x)=0$ everywhere inside the box. Thereofore, there will be no admissible particle with zero energy within the box.

Normalization of the wave function:

The wave function ψ_n corresponding to n^{th} quantum state is

$$\psi_n(x)=A\sin\frac{n\pi x}{a} \quad 0\le x\le a$$
$$=0 \qquad \text{otherwise}$$

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Since, the particle must be somewhere within the box, the total probability of finding the particle inside the box is unity i.e.

$$\int_0^a \psi_n^*(x)\psi_n(x)\,dx=1 \qquad \Rightarrow \int_0^a A^2\sin^2\frac{n\pi x}{a}dx=1$$

$$\Rightarrow A^2\int_0^a\frac{1}{2}\left[1-\cos\frac{2\pi nx}{a}\right]dx=1 \Rightarrow A=\sqrt{\frac{2}{a}}$$

Therefore, the normallized wave function will be

$$\psi_n(x)=\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right) \qquad (n=1,2,3,.....)$$

Energy eigenvalues:

We know that, $k=\sqrt{\frac{2mE}{\hbar^2}} \Rightarrow \frac{n^2\pi^2}{a^2}=\frac{2mE}{\hbar^2} \Rightarrow E_n=\frac{n^2\pi^2\hbar^2}{2ma^2} \quad (n=1,2,3,.....)$

So, we get an infinite sequence of descrete energy levels that corresponds to all integral values of n, where n is called the quantum number representing the different states of the particle.

Ground state energy: $n=1 \quad \Rightarrow E_1 = \dfrac{\pi^2\hbar^2}{2ma^2}$

First excited state energy: $n=2 \quad \Rightarrow E_2 = \dfrac{4\pi^2\hbar^2}{2ma^2}$

In general, $E_n = n^2 E_1$

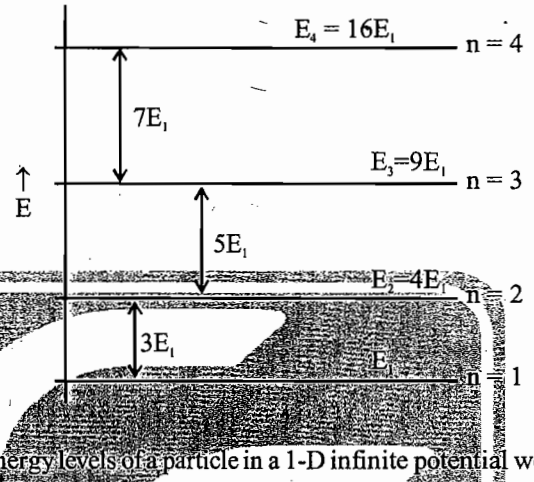


Figure : Energy levels of a particle in a 1-D infinite potential well

Difference between two consecutive energy levels

$$\Delta E_n = E_{n+1} - E_n = \frac{\pi^2\hbar^2}{2ma^2}\left[(n+1)^2 - n^2\right] = \frac{\pi^2\hbar^2}{2ma^2}(2n+1)$$

Spacing between two energy levels increases with 'n', decreases with size of the box 'a' and the mass of the particle 'm'. As $a \to \infty \Rightarrow \Delta E_n = 0$ i.e. the energy levels gets closer, forming a continuum of energy.

Momentum eigenvalues:

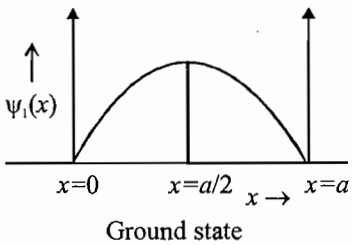
$$E_n = \frac{p_n^2}{2m} \Rightarrow P_n^2 = 2mE_n = 2m\frac{n^2\pi^2\hbar^2}{2ma^2} = \frac{n^2\pi^2\hbar^2}{a^2} \Rightarrow P_n = \pm\frac{n\pi\hbar}{a}$$

where '$\pm$' sign is due to the back and forth motion of the particle within the box.

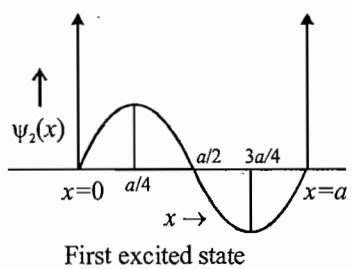
Difference of momentum between two consecutive energy levels

$$\Delta P_n = P_{n+1} - P_n = \pm\left[\frac{(n+1)\pi\hbar}{a} - \frac{n\pi\hbar}{a}\right] = \pm\frac{\pi\hbar}{a}$$

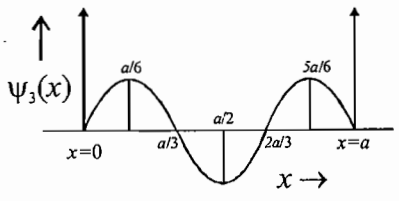
Various eigenstates of the particle inside a 1-D box :



Ground state



First excited state



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Note: $\psi_n(x)$ has $(n-1)$ nodes (excluding the boundary at $x = 0$ and $x = a$)

Variation of probability density corresponding to various eigenstates of the particle:

Probability density of finding the particle in the n[th] quantum state is given by,

$$P_n(x) = |\psi_n(x)|^2 = \frac{2}{a}\sin^2\frac{n\pi x}{a}$$

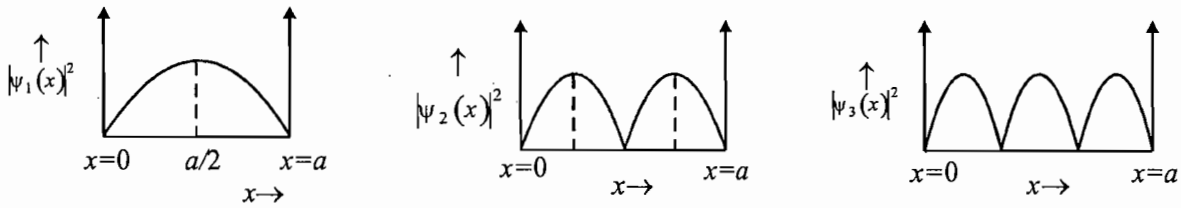

Figure : Variation of probability density corresponding to ground, first excited and second excited state respectively

Note:

(1) Probability of finding the particle in the left half of the well = Probability of finding the particle in the left half of the well = 1/2, for any state n.

(2) Probability of finding the particle between $\frac{a}{4} \le x \le \frac{3a}{4}$ is 1/2 for $n = 2, 4, 6, \ldots\ldots$

- The energy eigenfunctions of the particle confined in a 1-D box, satisfies the orthonormality condition i.e.

$$\int_0^a \psi_m^*(x)\psi_n(x)dx = \delta_{mn}$$

- As the energy eigenfunctions form a complete set, an arbitary function $\psi(x)$ (which is well behaved and satisfy the same boundary conditions) can be expanded in terms of these eigenfunctions as

$$\psi(x) = \sum_{n=1}^{\infty} c_n \psi_n(x) = \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)$$

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Expectation values of $\hat{x}, \hat{p}_x, \hat{x}^2, \hat{p}_x^2$:

$$\langle x\rangle = \int_0^a \psi^* x\psi\, dx = \int_0^a \frac{2}{a} x\sin^2\left(\frac{n\pi x}{a}\right)dx = \frac{2}{a}\int_0^a x\left[\frac{1-\cos\left(\frac{2n\pi x}{a}\right)}{2}\right]dx$$

$$= \frac{2}{a}\frac{1}{2}\left[\frac{x^2}{2} - x\frac{\sin\frac{2\pi nx}{a}}{\frac{2\pi n}{a}} - \cos\frac{2n\pi x}{a}\right]_0^a = \frac{1}{a}\left[\frac{a^2}{2} - 1 + 1\right] = \frac{a}{2}$$

Soln.

$$\langle p\rangle = \int_0^a \psi^*\left(-i\hbar\frac{\partial}{\partial x}\right)\psi\, dx = \frac{2}{a}(-i\hbar)\int_0^a \sin\left(\frac{n\pi x}{a}\right)\frac{n\pi}{a}\cos\left(\frac{n\pi x}{a}\right)dx = 0$$

Note: Expectation value of momentum for a real wave function is always zero.

$$\langle x^2\rangle = \int_0^a \psi^* x^2\,\psi\, dx = \frac{2}{a}\int_0^a x^2\sin^2\frac{n\pi x}{a}dx$$

$$= \frac{1}{a}\left[\left(\frac{x^3}{3}\right)_0^a - \left(x^2 \frac{\sin 2n\pi x/a}{2n\pi/a}\right)_0^a + \int_0^a 2x.\sin\frac{2n\pi x/a}{2n\pi/a}dx\right]$$

$$= \frac{1}{a}\left[\frac{a^3}{3} - 0 + 2\left\{-x\frac{\cos\frac{2n\pi x}{a}}{\left(\frac{2n\pi}{a}\right)^2} + \frac{\sin\frac{2n\pi x}{a}}{\left(\frac{2n\pi}{a}\right)^2}\right\}_0^a\right] = \frac{1}{a}\left[\frac{a^3}{3} - \frac{a^3}{2(n\pi)^2}\right] = \frac{a^2}{3} - \frac{a^2}{2n^2\pi^2}$$

$$\langle p^2\rangle = \frac{2}{a}\int_0^a \sin\left(\frac{n\pi x}{a}\right)\left(-\hbar^2\frac{\partial^2}{\partial x^2}\right)\sin\left(\frac{n\pi x}{a}\right)dx = \frac{2}{a}\left(-\hbar^2\right)\left(\frac{n\pi}{a}\right)^2(-1)\int_0^a \sin^2\left(\frac{n\pi x}{a}\right)dx$$

$$= \frac{2}{a}\left(-\hbar^2\right)\left(\frac{n\pi}{a}\right)^2(-1)\int_0^a \sin^2\left(\frac{n\pi x}{a}\right)dx$$

$$= \frac{n^2\pi^2\hbar^2}{a^2}\int_0^a\left[1-\cos\left(\frac{2n\pi x}{a}\right)\right]dx = \frac{n^2\pi^2\hbar^2}{a^2}\left[x - \frac{\sin\frac{2n\pi x}{a}}{\frac{2n\pi}{a}}\right]_0^a = \frac{n^2\pi^2\hbar^2}{a^2}$$

Uncertainity in the position of the particle is

$$\Delta x = \left[\langle x^2\rangle - \langle x\rangle^2\right]^{1/2} = \left[\frac{a^2}{3} - \frac{a^2}{2n^2\pi^2} - \frac{a^2}{4}\right]^{1/2} = \left[\frac{a^2}{12} - \frac{a^2}{2n^2\pi^2}\right]^{1/2}$$

Uncertainity in the momentum of the particle is

$$\Delta p = \left[\langle p^2\rangle - \langle p\rangle^2\right]^{1/2} = \frac{n\pi\hbar}{a}$$

Therefore, the uncertainity product $\Delta x\Delta p = n\pi\hbar\left[\frac{1}{12} - \frac{1}{2n^2\pi^2}\right]^{1/2}$

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Example 1: A particle in a deep square well potential extending from $x = 0$ to $x = L$ has a wave function $\psi(x) = \frac{1}{\sqrt{5}}\left[|\phi_1\rangle + 2|\phi_2\rangle\right]$ where $|\phi_1\rangle$ and $|\phi_2\rangle$ denote the ground state and the first excited state wave functions. Find the expectation of 'x' in this state.

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Soln. $\langle x\rangle = \langle\psi|x|\psi\rangle = \frac{1}{\sqrt{5}}\left(\langle\phi_1| + 2\langle\phi_2|\right)x\frac{1}{\sqrt{5}}\left(|\phi_1\rangle + 2|\phi_2\rangle\right)$

$$= \frac{1}{5}\left[\langle\phi_1|x|\phi_1\rangle + 2\langle\phi_1|x|\phi_2\rangle + 2\langle\phi_2|x|\phi_1\rangle + 4\langle\phi_2|x|\phi_2\rangle\right]$$

Now, $\langle\phi_1|X|\phi_2\rangle = \int_0^L\left(\sqrt{\frac{2}{L}}\sin\frac{\pi x}{L}\right)x\left(\sqrt{\frac{2}{L}}\sin\frac{2\pi x}{L}\right)dx$

$$= \frac{1}{L}\int_0^L x\left(\cos\frac{\pi x}{L} - \cos\frac{3\pi x}{L}\right)dx = \frac{1}{L}\left(-\frac{2L^2}{\pi^2} + \frac{2L^2}{9\pi^2}\right) = -\frac{16L}{9\pi^2}$$

Therefore, $\langle x\rangle = \frac{1}{5}\left[\frac{L}{2} - \frac{32L}{9\pi^2} - \frac{32L}{9\pi^2} + 4.\frac{L}{2}\right] = \frac{L}{2} - \frac{64L}{45\pi^2}$

Example 2: Calculate $\langle p_x\rangle$ for $\psi(x) = \frac{1}{\sqrt{2}}\left(|\phi_1\rangle + |\phi_2\rangle\right)$ where $|\phi_1\rangle$ and $|\phi_2\rangle$ are the ground state and the first excited state wave functions of a particle in a deep square well potential.

Soln. $\langle p_x\rangle = \langle\psi|p_x|\psi\rangle = \frac{1}{2}\left[\langle\phi_1|p_x|\phi_1\rangle + \langle\phi_2|p_x|\phi_1\rangle + \langle\phi_1|p_x|\phi_2\rangle + \langle\phi_2|p_x|\phi_2\rangle\right]$

$$\langle\phi_2|p_x|\phi_1\rangle = \int_{-\infty}^{\infty}\phi_2^*\left(-i\hbar\frac{d}{dx}\right)\phi_1(x)\,dx = \frac{2}{L}(-i\hbar)\int_0^L \sin\frac{2\pi x}{L}\frac{d}{dx}\left(\sin\frac{\pi x}{L}\right)dx$$

$$= \frac{-i\hbar\pi}{L^2}\int_0^L 2\sin\frac{2\pi x}{L}\cos\frac{\pi x}{L}\,dx = \frac{-i\hbar\pi}{L^2}\int_0^L\left(\sin\frac{3\pi x}{L} + \sin\frac{\pi x}{L}\right)dx = -\frac{8i\hbar}{3L}$$

Similarly, $\langle\phi_1|p_x|\phi_2\rangle = \frac{8i\hbar}{3L}$

Therefore, $\langle p_x\rangle = 0$

Example 3: The wave function of a particle in a deep square well potential extending from $x = 0$ to $x = L$ is $\psi(x) = \sqrt{30}\,x(x-L)/L^i$. (a) Find the value of i, (b) Find the average value of 'x' in this state.

Soln. (a) Any wave function of a particle in one dimension has the dimensions of $\frac{1}{\sqrt{L}}$. Thus $i = \frac{5}{2}$

(b) $\langle x\rangle = \int_{-\infty}^{\infty}\psi^*(x)\,x\psi(x)\,dx = \frac{30}{L^5}\int_0^L x^3(x-L)^2\,dx = \frac{L}{2}$

Example 4: A particle is in the ground state of a deep square well in the range $0 < x < L$. Suddenly the wall $x = L$ of the well is shifted to $x = 2L$, so as to make it a deep square well in the range $0 < x < 2L$. Immediately after this, the energy of the particle is measured. What will be the probability of getting the energy as the new ground state energy?

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Soln. The wave function just before the shifting of the wall is

$$\psi(x) = \sqrt{\frac{2}{L}}\sin\frac{\pi x}{L} \text{ for } 0 < x < L$$
$$= 0 \qquad \text{otherwise}$$

This is the energy eigenfunction corresponding to the ground state in the original well. When the wall is shifted, the new ground state wave function becomes,

$$\phi(x) = \sqrt{\frac{2}{2L}}\sin\frac{\pi x}{2L} \text{ for } 0 < x < 2L$$
$$= 0 \qquad \text{otherwise}$$

The probability of getting the ground state energy in measurements is $|\langle\phi|\psi\rangle|^2$

$$\langle\phi|\psi\rangle = \int_{-\infty}^{\infty} \phi^*(x)\psi(x)dx = \int_0^L \sqrt{\frac{2}{2L}}\sin\frac{\pi x}{2L}\sqrt{\frac{2}{L}}\sin\frac{\pi x}{L}dx$$

$$= \frac{1}{L\sqrt{2}}\int_0^L\left(\cos\frac{\pi x}{2L} - \cos\frac{3\pi x}{2L}\right)dx = \frac{1}{L\sqrt{2}}\left|\frac{\sin\frac{\pi x}{2L}}{\frac{\pi}{2L}} - \frac{\sin\frac{3\pi x}{2L}}{\frac{3\pi}{2L}}\right|_0^L = \frac{8}{3\sqrt{2}\,\pi}$$

Therefore, the probability is $|\langle\phi|\psi\rangle|^2 = \frac{32}{9\pi^2}$

Example 5: Consider a particle of mass 10^{-30} kg trapped in an infinitely deep potential well of width 0.5 nm. (a) Find the value of the wave number 'k' in the ground state. (b) How many states are there having value of 'k' between 10 nm^{-1} and 100 nm^{-1} ?

Soln. (a) $k = \frac{n\pi}{L}$. In ground state, $k = \frac{\pi}{L} = \frac{3.14}{0.5nm} = 6.28\ nm^{-1}$

(b) For every interval $\frac{\pi}{L}$ of k, there is one quantum state.

The total k-interval is, $\Delta k = 100\ nm^{-1} - 10\ nm^{-1} = 90\ nm^{-1}$

So, the number of states with 'k' value in the given interval is, $\frac{90\ nm^{-1}}{6.28\ nm^{-1}} = 14.33$

There are 14 states in the given interval.

Example 6: A particle of mass 'm' which moves freely inside an infinite potential well of width 'a' has the following wave fn (at t = 0)

$$\psi(x,0) = \frac{A}{\sqrt{a}}\sin\left(\frac{\pi x}{a}\right) + \sqrt{\frac{3}{5a}}\sin\left(\frac{3\pi x}{a}\right) + \frac{1}{\sqrt{5a}}\sin\left(\frac{5\pi x}{a}\right) \qquad [A = \text{real constant}]$$

(a) Find the value of A such that $\psi(x,0)$ is normalized to unity.

(b) If the measurement is carried out, what values will be found and with what probability? and also calculate $\langle E\rangle$

(c) Find the wavefunction $\psi(x,t)$

(d) Determine the probability of finding the system at time 't' in the state $\phi(x,t) = \sqrt{\frac{2}{a}}\sin\left(\frac{5\pi x}{a}\right)e^{-iE_5\frac{t}{\hbar}}$

Soln. (a) $\psi(x,0) = \frac{A}{\sqrt{2}}\sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right) + \sqrt{\frac{3}{10}}\sqrt{\frac{2}{a}}\sin\left(\frac{3\pi x}{a}\right) + \frac{1}{\sqrt{10}}\sqrt{\frac{2}{a}}\sin\left(\frac{5\pi x}{a}\right)$

$$\Rightarrow \quad \psi(x,0) = \frac{A}{\sqrt{2}}|\phi_1\rangle + \sqrt{\frac{3}{10}}|\phi_3\rangle + \frac{1}{\sqrt{10}}|\phi_5\rangle$$

Normalization condition: $\langle\psi(x,0)|\psi(x,0)\rangle = 1 \ \Rightarrow \ \sum_{n=1,3,5}|C_n|^2 = 1$

$$\Rightarrow \frac{A^2}{2} + \frac{3}{10} + \frac{1}{10} = 1 \ \Rightarrow A^2 = \frac{6}{5} \Rightarrow A = \sqrt{\frac{6}{5}}$$

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Therefore, $$|\psi(x,0)\rangle = \sqrt{\frac{6}{10}}|\phi_1\rangle + \sqrt{\frac{3}{10}}|\phi_3\rangle + \sqrt{\frac{1}{10}}|\phi_5\rangle$$

(b) The state of the particle is a linear combination of ground state $|\phi_1\rangle$, 2nd excited state $|\phi_3\rangle$ and 4th excited state $|\phi_5\rangle$ respectively. Therefore, the energies we will get are

$$E_1 = \frac{\pi^2\hbar^2}{2ma^2}, E_3 = \frac{9\pi^2\hbar^2}{2ma^2}, E_5 = \frac{25\pi^2\hbar^2}{2ma^2}$$

Now, the respective probabilties are

$$P(E_1) = |\langle\phi_1|\psi\rangle|^2 = \frac{3}{5}; \qquad P(E_2) = |\langle\phi_2|\psi\rangle|^2 = \frac{3}{10}; \qquad P(E_1) = |\langle\phi_3|\psi\rangle|^2 = \frac{1}{10}$$

$$\langle E\rangle = P(E_1).E_1 + P(E_3).E_3 + P(E_5).E_5$$

$$= \frac{3}{5}.\frac{\pi^2\hbar^2}{2ma^2} + \frac{3}{10}\frac{9\pi^2\hbar^2}{2ma^2} + \frac{1}{10}\frac{25\pi^2\hbar^2}{2ma^2}$$

$$= \frac{\pi^2\hbar^2}{2ma^2}\left[\frac{3}{5} + \frac{27}{10} + \frac{5}{2}\right] = \frac{29\pi^2\hbar^2}{10ma^2}$$

(c) $$|\psi(x,t)\rangle = \sqrt{\frac{6}{10}}|\phi_1\rangle e^{-iE_1 t/\hbar} + \sqrt{\frac{3}{10}}|\phi_3\rangle e^{-iE_3 t/\hbar} + \sqrt{\frac{1}{10}}|\phi_5\rangle e^{-iE_5 t/\hbar}$$

(d) $$|\phi(x,t)\rangle = |\phi_5\rangle e^{-iE_5 t/\hbar} \quad \Rightarrow \quad P = |\langle\phi(x,t)|\psi\rangle|^2 = \frac{1}{10}$$

Example 7: A particle of mass m confined to move in a potential $V(x) = 0$ for $0 \le x \le a$ and $V(x) = \infty$ otherwise. The wave function of the particle at time $t = 0$ is

$\psi(x,0) = A\left(2\sin\frac{\pi x}{a} + \sin\frac{3\pi x}{a}\right)$ (i) Normalize $\psi(x,0)$; (ii) find $\psi(x,t)$.

Soln. For a particle, in the potential given, the energy eigenvalues and eigenfunctions are given by

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}, \psi_n(x) = \sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a}, \quad n = 1, 2, 3, ...$$

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(i) Normalization condition: $\int_0^a \psi^*\psi dx = 1 \Rightarrow A^2\int_0^a\left(2\sin\frac{\pi x}{a} + \sin\frac{3\pi x}{a}\right)^2 dx = 1$

$$\Rightarrow A^2\left(4\frac{a}{2} + \frac{a}{2}\right) = 1 \Rightarrow A = \sqrt{\frac{2}{5a}}$$

Therefore, $\psi(x,0) = \frac{1}{\sqrt{5}}\left(2\sqrt{\frac{2}{a}}\sin\frac{\pi x}{a} + \sqrt{\frac{2}{a}}\sin\frac{3\pi x}{a}\right) = \frac{1}{\sqrt{5}}(2\psi_1 + \psi_3)$

(ii) $\psi(x,t) = \frac{1}{\sqrt{5}}(2\psi_1 e^{-iE_1 t/\hbar} + \psi_3 e^{-iE_3 t/\hbar})$

Example 8: A particle in a box is in a superposition state and is described by the wave function

$$\psi(x,t)=\frac{1}{\sqrt{a}}\left[\exp\left(\frac{-iE_1t}{\hbar}\right)\cos\frac{\pi x}{2a}+\exp\left(\frac{-iE_2t}{\hbar}\right)\sin\frac{2\pi x}{2a}\right],\qquad -a<x<a$$

where E_1 and E_2 are the energy eigenvalues of the first two states. Find the expectation value of x.

Soln. $\langle x\rangle=\int_{-\infty}^{\infty}\psi^*(x,t)x\psi(x,t)dx=\frac{1}{a}\int_{-a}^{a}x\cos^2\frac{\pi x}{2a}dx+\frac{1}{a}\int_{-a}^{a}x\sin^2\frac{2\pi x}{2a}dx$

$$+\frac{1}{a}\{\exp[i(E_1-E_2)t/\hbar)]+\exp[i(E_2-E_1)t/\hbar)]\}\int_{-a}^{a}x\cos\frac{\pi x}{2a}\sin\frac{2\pi x}{2a}dx$$

The integrands in the first two terms are odd and hence will not contribute.

$$\int_{-a}^{a}x\cos\frac{\pi x}{2a}\sin\frac{2\pi x}{2a}dx=\int_{-a}^{a}\frac{x}{2}\left(\sin\frac{3\pi x}{2a}+\sin\frac{\pi x}{2a}\right)dx=\frac{1}{2}\left[-\frac{8a^2}{9\pi^2}+\frac{8a^2}{\pi^2}\right]=\frac{32a^2}{9\pi^2}$$

Therefore,

$$\langle x\rangle=\frac{2}{a}\cos\frac{(E_2-E_1)t}{\hbar}\left(\frac{32a^2}{9\pi^2}\right)=\frac{64a}{9\pi^2}\cos\frac{(E_2-E_1)t}{\hbar}$$

Example 9: For an electron in a one-dimensional infinite potential well of width 1Å, calculate (i) the separation between the two lowest energy levels; (ii) the frequency and wavelength of the photon corresponding to a transition between these two levels; and (iii) in what region of the electromagnetic spectrum is this frequency / wavelength?

Soln. (i) Energy of the particle in the nth state $E_n=\frac{\pi^2\hbar^2n^2}{2ma^2}$

Separation between two lowest enegy states will be

$$E_2-E_1=\frac{3\pi^2\hbar^2}{2ma^2}=113.27\text{eV}$$

(ii) Frequency of the photon $\nu=\frac{E}{\hbar}=2.7\times10^{16}\ Hz$

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Wavelength of the photon $\lambda=\frac{c}{\nu}=\frac{3\times10^8\,\text{ms}^{-1}}{2.7\times10^{16}\,\text{s}^{-1}}=1.1\times10^{-8}\,\text{m}$

(iii) This frequency falls in the vacuum ultraviolet region.

Example 10: A particle of mass m trapped in the potential $V(x)=0$ for $-a\le x\le a$ and $V(x)=\infty$ otherwise. Evaluate the probability of finding the trapped particle between $x=0$ and $x=a/n$ when it is in the nth state.

Soln. Wave function $\psi_n(x)=\sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a}$

Required probability $P=\int_0^{a/n}\psi_n^*\psi_n dx=\frac{2}{a}\int_0^{a/n}\sin^2\frac{n\pi x}{a}dx\frac{1}{a}\int_0^{a/n}\left(1-\cos\frac{2n\pi x}{a}\right)dx=\frac{1}{n}$

Example 11: An electron is in the ground state of a one-dimensional infinite square well with $a = 10^{-10}$ m. Compute the force that the electron exerts on the wall during an impact on either wall.

Soln. The force on the wall $F = -\dfrac{dE_n}{da}$

The energy of the ground state $E_1 = \dfrac{\pi^2\hbar^2}{2ma^2}$

and hence the force on the wall $F = -\left.\dfrac{dE_1}{da}\right|_{a=10^{-10}m} = \left.\dfrac{\pi^2\hbar^2}{ma^3}\right|_{a=10^{-10}m} = 1.21\times10^{-7}N$

3.3 One-dimensional finite potential well:

Consider a particle of mass '*m*' and energy $E\,(<V_0)$ is moving along x-axis, in the region from $x = 0$ to $x = a$ under the following potential i.e.

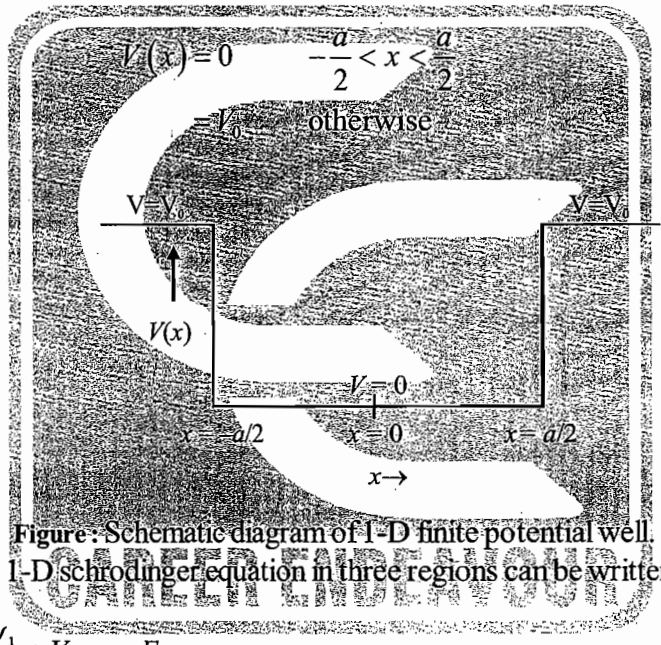

Figure: Schematic diagram of 1-D finite potential well.

The time independent 1-D schrodinger equation in three regions can be written as

Region-1: $-\dfrac{\hbar^2}{2m}\dfrac{d^2\psi_1}{dx^2} + V_0\psi_1 = E\psi_1$ (5a)

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Region-2: $-\dfrac{\hbar^2}{2m}\dfrac{d^2\psi_2}{dx^2} = E\psi_2$ (5b)

Region-3: $-\dfrac{\hbar^2}{2m}\dfrac{d^2\psi}{dx^2} + V_0\psi_3 = E\psi_3$ (5c)

Aasuming $\alpha^2 = \dfrac{2m(V_0 - E)}{\hbar^2}$ and $\beta^2 = \dfrac{2mE}{\hbar^2}$, equations (5a), (5b) and (5c) can be written as

Region-1: $\dfrac{d^2\psi_1}{dx^2} - \alpha^2\psi_1 = 0$ (6a)

Region-2: $\dfrac{d^2\psi_2}{dx^2} + \beta^2\psi_2 = 0$ (6b)

Region-3: $\frac{d^2\psi_3}{dx^2} - \alpha^2\psi_3 = 0$ (6c)

Solution of equations (6a), (6b) and (6c) will be of the following form:

$$\psi_1(x) = Ae^{\alpha x} + Be^{-\alpha x} \qquad \left(x \le -\frac{a}{2}\right)$$

$$\psi_2(x) = C\cos\beta x + D\sin\beta x \quad \left(-\frac{a}{2} < x < \frac{a}{2}\right)$$

$$\psi_3(x) = F\,e^{-\alpha x} + G\,e^{\alpha x} \qquad \left(x \ge \frac{a}{2}\right)$$

Boundary conditions:

(i) $\psi(x) \to 0$ at $x \to \pm\infty$ (ii) $\psi(x)$ and $\frac{d\psi}{dx}$ are continuous at $x = \pm\frac{a}{2}$

Using the first condition, we get B = 0 and G = 0.

Since the particle is moving under a symmetric potential, then the wavefunction of the particle should have a definite parity i.e. either even or odd.

(1) Even bound states:

The wave function of the particle will be of the form:

$$\psi_1(x) = Ae^{\alpha x} \qquad \left(x \le -\frac{a}{2}\right)$$

$$\psi_2(x) = C\cos\beta x \qquad \left(-\frac{a}{2} < x < \frac{a}{2}\right)$$

$$\psi_3(x) = F\,e^{-\alpha x} \qquad \left(x \ge \frac{a}{2}\right)$$

Now, boundary conditions are

$$\psi_1\left(x = -\frac{a}{2}\right) = \psi_2\left(x = -\frac{a}{2}\right) \Rightarrow Ae^{-\alpha\frac{a}{2}} = C\cos\beta\frac{a}{2} \tag{9}$$

$$\frac{d\psi_1}{dx}\left(x = -\frac{a}{2}\right) = \frac{d\psi_2}{dx}\left(x = -\frac{a}{2}\right) \Rightarrow \alpha Ae^{-\alpha\frac{a}{2}} = \beta C\sin\beta\frac{a}{2} \tag{10}$$

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Dividing equation (10) by (9), we get, $\beta\tan\beta\frac{a}{2} = \alpha$ (11)

We know that, $\alpha^2 + \beta^2 = \frac{2mV_0}{\hbar^2}$ (12)

Defining $\beta\frac{a}{2} = p$ and $\alpha\frac{a}{2} = q$, we get

$$p\tan p = q \text{ and } p^2 + q^2 = \frac{mV_0a^2}{2\hbar^2} \tag{13}$$

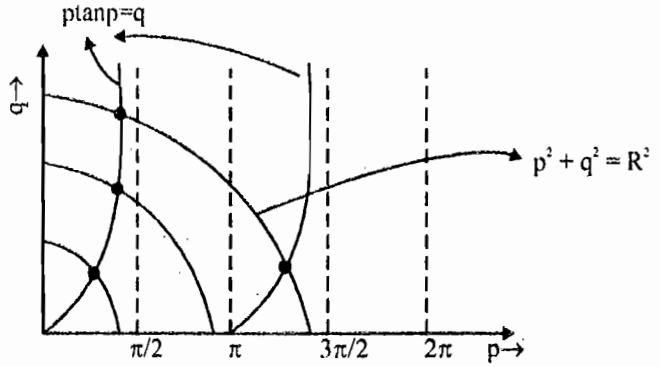
The second equation represents a circle in the p-q plane with radius $R = \sqrt{\frac{mV_0a^2}{2\hbar^2}}$ which depends upon the the height V_0 and width a of the finite potential well. Both of these can be solved graphically and the points of

intersection of the curves $p\tan$ ... $\frac{mV_0a^2}{2\hbar^2}$

$$p_n = p_0, p_2, p_4, \ldots\ldots$$

which also gives the discrete spectrum of energy values for the even eigenstates as

$$E_n = \frac{2\hbar^2 p^2}{ma^2} \quad (n = 0,2,4,6\ldots\ldots)$$



Number of even bound states:

$0 < R < \pi \Rightarrow$ one even bound state

$\pi < R < 2\pi \Rightarrow$ two even bound state

In general, $n\pi < R < (n+1)\pi \Rightarrow (n+1)$ even bound state

(2) Odd bound states:

The wave function of the particle will be of the form:

$$\psi_1(x) = Ae^{\alpha x} \qquad \left(x \le -\frac{a}{2}\right)$$

$$\psi_2(x) = D\sin\beta x \qquad \left(-\frac{a}{2} < x < \frac{a}{2}\right)$$

$$\psi_3(x) = F e^{-\alpha x} \qquad \left(x \ge \frac{a}{2}\right)$$

Now, boundary conditions are

$$\psi_1\left(x = -\frac{a}{2}\right) = \psi_2\left(x = -\frac{a}{2}\right) \Rightarrow Ae^{-\alpha\frac{a}{2}} = -D\sin\beta\frac{a}{2} \tag{15}$$

$$\frac{d\psi_1}{dx}\left(x = -\frac{a}{2}\right) = \frac{d\psi_2}{dx}\left(x = -\frac{a}{2}\right) \Rightarrow \alpha Ae^{-\alpha\frac{a}{2}} = \beta D\cos\beta\frac{a}{2} \tag{16}$$

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Dividing equation (10) by (9), we get, $\beta\cot\beta\frac{a}{2} = -\alpha$ (17)

We know that, $\alpha^2 + \beta^2 = \frac{2mV_0}{\hbar^2}$ (18)

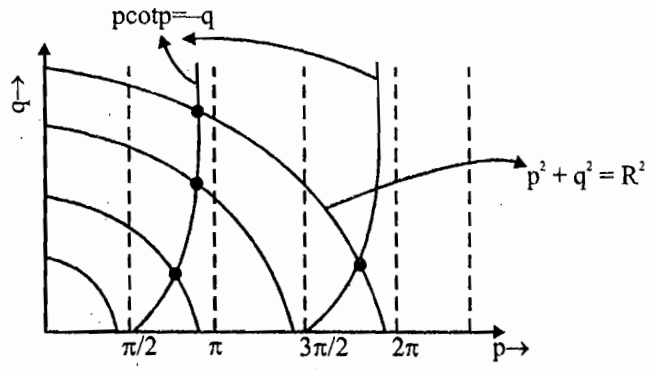
Defining $\beta\frac{a}{2} = p$ and $\alpha\frac{a}{2} = q$, we get

$$p\cot p = -q \text{ and } p^2 + q^2 = \frac{mV_0a^2}{2\hbar^2} \tag{19}$$

Both of these can be solved graphically and the points of intersection of the curves $p\cot p = -q$ and $p^2 + q^2 = \frac{mV_0a^2}{2\hbar^2}$ gives different p values i.e.

which also gives the discrete spectrum of energy values for the even eigenstates as

$$E_n = \frac{2\hbar^2 p^2}{ma^2} \quad (n = 1,3,5,7.....)$$



Number of Odd bound states:

$\frac{\pi}{2} < R < \frac{3\pi}{2} \Rightarrow$ one odd bound state

$\frac{3\pi}{2} < R < \frac{5\pi}{2} \Rightarrow$ two odd bound state

In general, $(2n-1)\frac{\pi}{2} < R < (2n+1)\frac{\pi}{2} \Rightarrow n$ odd bound state

Range of R	No. of bound states	Even	Odd
$0 < R < \frac{\pi}{2}$	1	1	0
$\frac{\pi}{2} < R < \pi$	2	1	1
$\pi < R < \frac{3\pi}{2}$	3	2	1
$\frac{3\pi}{2} < R < 2\pi$	4	2	2

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(15)

(16)

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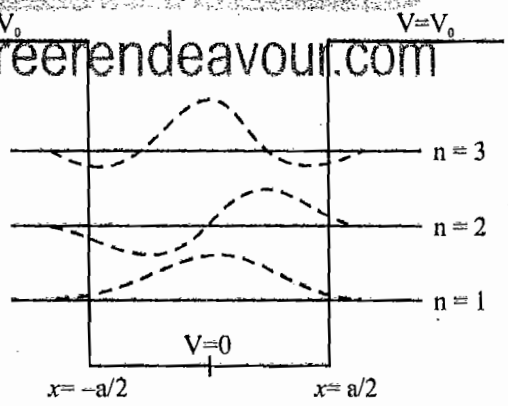
(17)

(18)



(19)

curve

Example 9: There are only 3 bound states for a particle of mass 'm' in a 1-D potential well of the form:

$$V(x) = 0 \qquad -\frac{a}{2} < x < \frac{a}{2}$$

$= V$ otherwise

The depth of the potential well satisfies the condition.

(a) $\frac{2\pi^2\hbar^2}{ma^2} < V_0 < \frac{9\pi^2\hbar^2}{2ma^2}$ (b) $\frac{2\pi^2\hbar^2}{2ma^2} < V_0 < \frac{4\pi^2\hbar^2}{2ma^2}$

(c) $\frac{2\pi^2\hbar^2}{2ma^2} < V_0 < \frac{8\pi^2\hbar^2}{ma^2}$ (d) $\frac{2\pi^2\hbar^2}{2ma^2} < V_0 < \frac{50\pi^2\hbar^2}{ma^2}$

Soln. For three bound states of the particle, $\pi < R < \frac{3\pi}{2}$

$$\Rightarrow \pi^2 < R^2 < \frac{9\pi^2}{4} \qquad \Rightarrow \pi^2 < \frac{mV_0a^2}{2\hbar^2} < \frac{9\pi^2}{4} \qquad \Rightarrow \frac{2\pi^2\hbar^2}{ma^2} < V_0 < \frac{9\pi^2\hbar^2}{2ma^2}$$

Example 10. Consider a particle of mass 'm' is confined to a finite potential will

$$V(x) = 0 \quad \text{if } |x| < L$$
$$= V_0 \quad \text{if } |x| \geq L$$

The particle is found to be in a bound state with energy $\frac{\pi^2\hbar^2}{32ma^2}$. The depth of the well is equal to

(a) $\frac{\pi^2\hbar^2}{2mL^2}$ (b) $\frac{\pi^2\hbar^2}{4mL^2}$ (c) $\frac{\pi^2\hbar^2}{8mL^2}$ (d) $\frac{\pi^2\hbar^2}{16mL^2}$

Soln. $\beta^2 = \frac{2mE}{\hbar^2} = \frac{\pi^2}{16L^2} \Rightarrow \beta = \frac{\pi}{4L}$

Since, the bound state is the ground state of the particle, therefore

$$\alpha = \beta\tan(\beta L) \Rightarrow \beta = \frac{\pi}{4L}\tan\left(\frac{\pi}{4}\right) = \frac{\pi}{4L}$$

Now, $\alpha^2 + \beta^2 = \frac{2mV_0}{\hbar^2} \Rightarrow V_0 = 2\frac{\pi^2}{16L^2} \times \frac{\hbar^2}{2m} = \frac{\pi^2\hbar^2}{16mL^2}$

Correct answer is (d)

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Example 11. Show that the ground state energy of a particle of mass 'm' in a finite square well potential of width L is less than that in infinite square well potential of the same width.

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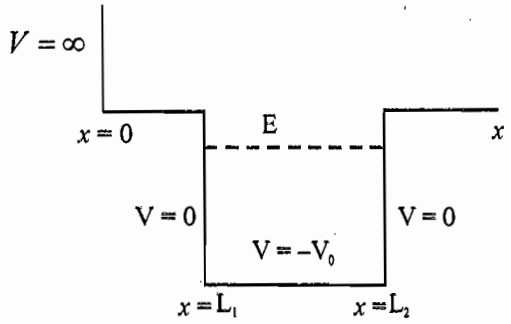
Soln. The ground state energy eigenvalue can be obtained from the intersection of the first branch of the curve $p\tan p = q$ and $p^2 + q^2 = \frac{mV_0L^2}{2\hbar^2}$. This point of intersection must corresponds to a value of p less than $\pi/2$.

This becuase at $p = \frac{\pi}{2}$, the function $q = p\tan p$ goes to infinity and for $p > \frac{\pi}{2}$, the first branch does not exists.

Therefore, $\frac{2mE}{\hbar^2}\frac{L^2}{4} < \frac{\pi^2}{4} \Rightarrow E < \frac{\pi^2\hbar^2}{2mL^2}$

Example 12. Consider a particle in a potential shown in figure below.



Write down the wave unctions of the particle (having energy eigenvalue E) in the different regions for bound states.

Soln. As is clear from the figure, the energy E should be negative for bound states. We can define four regions.

Region-I: $x<0$, **Region-II** : $0<x<L_1$, **Region-III**: $L_1<x<L_2$ and **Region-IV:** $x>L_2$. The wave function for a bound state at energy E can be written as, (solving 1-D time independent Schrodinger equation)

$$\phi_I(x)=0;\ \phi_{II}(x)=Ae^{\alpha x}+Be^{-\alpha x}$$

$$\phi_{III}(x)=C\sin\beta x+D\cos\beta x$$

$$\phi_{IV}(x)=Fe^{-\alpha x}$$

where, $\alpha=\sqrt{\dfrac{-2mE}{\hbar^2}}$ and $\beta=\sqrt{\dfrac{2m(V_0+E)}{\hbar^2}}$

Example 13. A particle is in its first excited state in a finite square well potential extended from $x=-\dfrac{L}{2}$ to $x=\dfrac{L}{2}$. The maximum value of the wave function, at a particular instant, is $\psi=A$ and it occurs at $x=\dfrac{L}{3}$. Find the value of the function at $x=\dfrac{L}{2}$.

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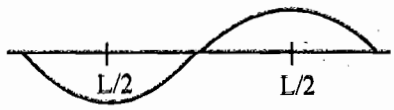
Soln. In the first excited state, the wave function is of the form $\psi=A\sin kx$. The maximum value of the wave function is A. According to the question, this occurs at $x=\dfrac{L}{3}$. This means,

$$A=A\sin\frac{kL}{3}\quad\Rightarrow\frac{kL}{3}=\frac{\pi}{2}\Rightarrow k=\frac{3\pi}{2L}$$



The wave function at $x=\dfrac{L}{2}$ is $\psi=A\sin\dfrac{kL}{2}=A\sin\left(\dfrac{3\pi}{2L}\times\dfrac{L}{2}\right)=\dfrac{A}{\sqrt{2}}$

Example 14. A finite square well potential has length L and depth V_0. A particle of mass $\dfrac{2\hbar^2}{V_0L^2}$ is trapped in this potential. Show that it has only one bound state and the energy corresponding to this states satisfies $\cos\left(\sqrt{E/V_0}\right)=\sqrt{E/V_0}$

Soln. $p^2+q^2=\left(\frac{L}{2}\right)^2\left[\frac{2mV_0}{\hbar^2}\right]=\frac{V_0L^2}{2\hbar^2}\times\frac{2\hbar^2}{V_0L^2}=1$

Thus, $\sqrt{p^2+q^2}<\frac{\pi}{2}$ and hence only one bound state occurs.

For the energy E, $q=p\tan p\Rightarrow\cos p=\frac{1}{\sqrt{1+\tan^2 p}}=\frac{p}{\sqrt{p^2+q^2}}=p$

Using, $p=\beta\frac{L}{2}=\frac{L}{2}\times\sqrt{\frac{2mE}{\hbar^2}}=\frac{L}{2}\sqrt{\frac{2E}{\hbar^2}\times\frac{2\hbar^2}{V_0L^2}}=\sqrt{\frac{E}{V_0}}$

Therefore, $\cos\left(\sqrt{\frac{E}{V_0}}\right)=\sqrt{\frac{E}{V_0}}$

3.4 One-dimensional step potential:

Let a particle of mass m and kinetic energy E is travelling parallel to the x-axis and is incident on the potential step at $x = 0$, given as following:

$$V(x)=\begin{cases}0 & \text{for } x<0\\ V_0 & \text{for } x\geq 0\end{cases}$$

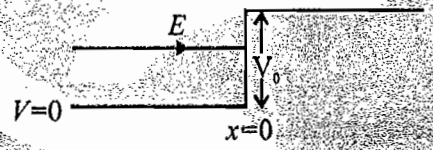


Figure : Schematic diagram of a 1-D step potential

The energy E of the particle is wholly kinetic for $x < 0$ and partly kinetic and partly potential for $x > 0$. From classical point of view in region I, the particle can move freely as $V(x) = 0$. If $E < V_0$, the particle will be reflected back at $x = 0$ and will remain in region I for ever. But for $E > V_0$ the particle will not be reflected back at $x = 0$ instead enter the region II.

Quantum mechanically, it will be shown that the electrons will be partly reflected and partly transmitted at x = 0. This is due to the wave nature of the moving particle.

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Case A: ($E > V_0$)

The time-independent Schrodinger equation for

Region 1: $-\frac{\hbar^2}{2m}\frac{d^2\psi_1}{dx^2}=E\psi_1 \Rightarrow \frac{d^2\psi_1}{dx^2}+\frac{2mE}{\hbar^2}\psi_1=0 \Rightarrow \frac{d^2\psi_1}{dx^2}+\alpha^2\psi_1=0$ (20)

Region 2: $-\frac{\hbar^2}{2m}\frac{d^2\psi_2}{dx^2}+V_0\psi_2=E\psi_2 \Rightarrow \frac{d^2\psi_2}{dx^2}+\frac{2m}{\hbar^2}(E-V_0)\psi_2=0 \Rightarrow \frac{d^2\psi_2}{dx^2}+\beta^2\psi_2=0$ (21)

where, $\alpha=\sqrt{\frac{2mE}{\hbar^2}}$ and $\beta=\sqrt{\frac{2m(E-V_0)}{\hbar^2}}$

The general solutions of equations are

... $A e^{i\alpha x}+B e^{-i\alpha x}$ ... $C e^{i\beta x}+D e^{-i\beta x}$ ... (22)

The terms $e^{i\alpha x}$ and $e^{-i\alpha x}$ represent respectively a wave travelling along the positive x-direction i.e. incident wave and a wave travelling along the negative x-direction, i.e., a reflected wave. Again, the terms $e^{i\beta x}$ and $e^{-i\beta x}$ represent respectively a wave travelling along the positive x-direction i.e transmitted wave and a wave travelling along the negative x-direction (a reflected wave). But due to the presence of only one discontinuity at $x = 0$, there cannot be any reflected waves in region II. Hence D = 0. Therefore,

Applying the following boundary conditions:

(i) $(\psi_1)_{x=0} = (\psi_2)_{x=0}$ and (ii) $\left(\frac{d\psi_1}{dx}\right)_{x=0} = \left(\frac{d\psi_2}{dx}\right)_{x=0}$

we will get, $B = \frac{\alpha-\beta}{\alpha+\beta}A$ and $C = \left(\frac{2\alpha}{\alpha+\beta}\right)A$

therefore, wavefunction in region 1 and region 2 will be

$$\psi_1 = A\left[e^{i\alpha x} + \left(\frac{\alpha-\beta}{\alpha+\beta}\right)e^{-i\alpha x}\right]$$

$$\psi_2 = \left(\frac{2\alpha}{\alpha+\beta}\right)Ae^{i\beta x} \qquad (23)$$

The probability current density for the incident beam of particles $J_i = \frac{\hbar\alpha}{m}|A|^2$

The probability current density for the reflected beam of particles $J_r = \frac{\hbar\alpha}{m}|B|^2$

The probability current density for the transmitted beam of particles $J_t = \frac{\hbar\beta}{m}|C|^2$

Using the relations between A, B and C we get,

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$$J_r + J_t = \frac{\hbar\alpha}{m}|A|^2\frac{(\alpha-\beta)^2}{(\alpha+\beta)^2} + \frac{4\alpha}{(\alpha+\beta)^2}\frac{\hbar\beta}{m}|A|^2 = \left[\frac{(\alpha-\beta)^2}{(\alpha+\beta)^2} + \frac{4\alpha\beta}{(\alpha+\beta)^2}\right]\frac{\hbar\alpha}{m}|A|^2$$

$$= \left[\frac{(\alpha-\beta)^2}{(\alpha+\beta)^2} + \frac{4\alpha\beta}{(\alpha+\beta)^2}\right]J_i \quad \Rightarrow \quad J_r + J_t = J_i$$

i.e. total number of particles is conserved in the process.

Reflection and Transmission Coefficients:

Reflection coefficient

$$R = \frac{\text{Reflected flux}\,(J_r)}{\text{Incident flux}\,(J_i)} = \frac{\frac{\hbar\alpha}{m}|B|^2}{\frac{\hbar\alpha}{m}|A|^2} = \frac{|B|^2}{|A|^2} = \left(\frac{\alpha-\beta}{\alpha+\beta}\right)^2 = \left(\frac{\sqrt{E}-\sqrt{E-V_0}}{\sqrt{E}+\sqrt{E-V_0}}\right)^2$$

Transmission coefficient

$$T = \frac{\text{Transmitted flux}\,(J_t)}{\text{Incident flux}\,(J_i)} = \frac{\frac{\hbar\beta}{m}|C|^2}{\frac{\hbar\alpha}{m}|A|^2} = \frac{\beta}{\alpha}\frac{|C|^2}{|A|^2} = \frac{4\alpha\beta}{(\alpha+\beta)^2} = \frac{4\sqrt{E(E-V_0)}}{\left(\sqrt{E}+\sqrt{E-V_0}\right)^2}$$

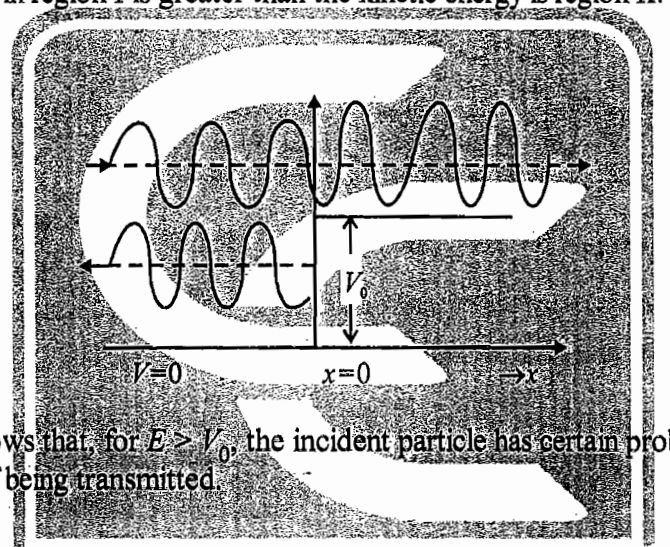
Note:

(i) $T + R = \frac{4\alpha\beta}{(\alpha+\beta)^2} + \frac{(\alpha-\beta)^2}{(\alpha+\beta)^2} = 1$

(ii) For $E = V_0$, $R = 1$ and $E >> V_0$, $R = 0$

(iii) For $E = V_0$, $T = 0$ and $E >> V_0$, $T = 1$

(iv) Amplitude (C) of the transmitted wave is greater than that of the incident wave (A) as $\alpha > \beta$. (v) De Broglie wavelength in region I will be shorter than that in region II. This is due to the fact that the kinetic energy of the particle in region I is greater than the kinetic energy is region II. The nature of the wave forms is shown in figure.



The analysis thus shows that, for $E > V_0$, the incident particle has certain probability of being reflected and certain probability of being transmitted.

Case B : ($E < V_0$)

The time-independent Schrodinger equation for

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Region 1: $-\frac{h^2}{2m}\frac{d^2\psi_1}{dx^2} = E\psi_1 \Rightarrow \frac{d^2\psi_1}{dx^2} + \frac{2mE}{\hbar^2}\psi_1 = 0 \Rightarrow \frac{d^2\psi_1}{dx^2} + \alpha^2\psi_1 = 0$ (24)

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Region 2: $-\frac{h^2}{2m}\frac{d^2\psi_1}{dx^2} + V_0\psi_1 = E\psi_1 \Rightarrow \frac{d^2\psi_2}{dx^2} + \frac{2m}{\hbar^2}(E-V_0)\psi_2 = 0 \Rightarrow \frac{d^2\psi_2}{dx^2} - \beta^2\psi_2 = 0$ (25)

where, $\alpha = \sqrt{\frac{2mE}{\hbar^2}}$ and $\beta = \sqrt{\frac{2m(V_0-E)}{\hbar^2}}$

The general solutions of equations are

$$\psi_1 = Ae^{i\alpha x} + Be^{-i\alpha x}, \quad \psi_2 = Ce^{\beta x} + De^{-\beta x} \tag{26}$$

But the term, $e^{\beta x} \to \infty$ as $x \to \infty$ which contradicts the condition of well-behaved wave function.

Therefore, C = 0.

Applying the following boundary conditions:

(i) $(\psi_1)_{x=0} = (\psi_2)_{x=0}$ and (ii) $\left(\frac{d\psi_1}{dx}\right)_{x=0} = \left(\frac{d\psi_2}{dx}\right)_{x=0}$

we will get, $B = \frac{i\alpha+\beta}{i\alpha-\beta}A$ and $D = \left(\frac{2i\alpha}{i\alpha-\beta}\right)A$

therefore, wavefunction in region 1 and region 2 will be

$$\psi_1 = A\left[e^{i\alpha x} + \left(\frac{i\alpha+\beta}{i\alpha-\beta}\right)e^{-i\alpha x}\right]$$

$$\psi_2 = \left(\frac{2i\alpha}{i\alpha-\beta}\right)Ae^{-\beta x} \qquad (27)$$

The probability current density for the incident beam of particles $J_i = \frac{\hbar\alpha}{m}|A|^2$

The probability current density for the reflected beam of particles $J_r = \frac{\hbar\alpha}{m}|B|^2$

The probability current density for the transmitted beam of particles $J_t = 0$

Using the relations between A, B and C we get, $J_i = J_r$

Reflection and Transmission Coefficients:

Reflection coefficient $R = \frac{\text{Reflected flux}(J_r)}{\text{Incident flux}(J_i)} = \frac{\frac{\hbar\alpha}{m}|B|^2}{\frac{\hbar\alpha}{m}|A|^2} = \frac{|B|^2}{|A|^2} = 1$

Hence, the incident wave is totally reflected at the potential step at $x = 0$.

Transmission coefficient $T = \frac{\text{Transmitted flux}(J_t)}{\text{Incident flux}(J_i)} = 0$

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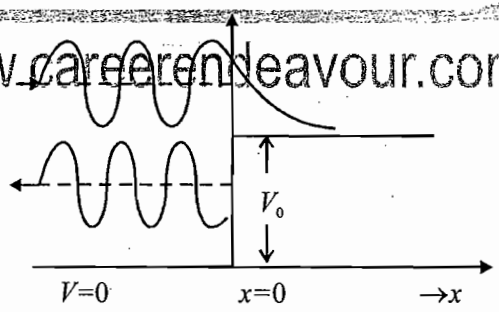


The phenomenon is very much similar to the case of total internal reflection of electromagnetic waves while travelling from denser to a rarer medium.

Quantam mechanically, the wave function of the particle in the region 2 is non-zero. therefore, the probability of finding the particle in classically forbidden region (region 2) is

$$P_2(x) = |\psi_2(x)|^2 = |D|^2 e^{-2\beta x}$$

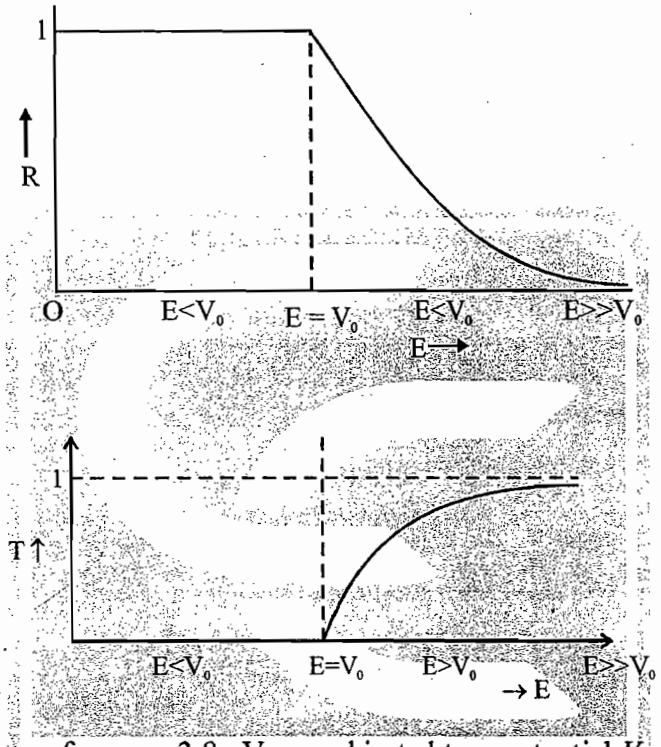
Such penetration of a barrier by a particle (having energy lower than barrier height), falls exponentially with distance from the step potential barrier.

Penetration depth:

It is defined as the distance at which wave function reduces to 1/e of the value of the wave function at the barrier (x = 0) and given by

$$x = \frac{1}{\beta} = \sqrt{\frac{\hbar^2}{2m(V_0 - E)}}$$

The fact that particle can penetrate into the classically forbidden region leads to Quantum Mechanical Tunnelling. If the potential barrier is infinitely high i.e. $V_0 \to \infty$, then penetration depth becomes very much negligible.



Example 15. Electrons of energy 3.8 eV are subjected to a potential $V = 0$ for $x < 0$ and $V = 7.6$ eV for $x > 0$. (a) Find the wavelength of the sinusoidal variation of the wave function in the classically allowed region (b) the reflected wave differs from the incident wave by a phase factor. Find this phase factor.

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Soln. **(a)** The wave number 'k' is $\alpha = \sqrt{\frac{2m_e E}{\hbar^2}} = \sqrt{\frac{3.8\ eV}{38 \times 10^{-3}\ eV\ nm^2}} = 10\ nm^{-1}$

The wavelength is $\lambda = \frac{2\pi}{\alpha} = \frac{6.28}{10\ nm^{-1}} \approx 0.63\ nm$

(b) The wave function in the classically allowed region is

$$\psi = A_1\left[e^{i\alpha x} + \frac{i\alpha + \beta}{i\alpha - \beta}e^{-i\alpha x}\right]$$

Thus the reflected wave differs from the incident wave by a phase factor $f = \frac{ik + \gamma}{ik - \gamma}$

We have $\alpha = 10\ nm^{-1}$ and similarly $\beta = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}} = 10\ nm^{-1}$. So, $f = e^{i\frac{3\pi}{2}}$

Example 16. Electrons of energy 10 eV are incident on a potential step of height 13.8 eV. Find the distance in which the probability density of finding the particle decreases to a factor of 0.01 as it penetrates into the classically forbidden region.

Soln. The wave function in the classically forbidden region is of the form

$$\psi = C e^{-\beta x}$$

where, $\beta = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}} = \sqrt{\frac{(13.8-10)eV}{38\times10^{-3}\ eV\ nm^2}} = 10\ nm^{-1}$

According to the question,

$$P(x+d) = 0.01P(x) \Rightarrow |C|^2 e^{-2\gamma(x+d)} = 0.01|C|^2 e^{-2\gamma x}$$

$$\Rightarrow e^{2\gamma d} = 100 \Rightarrow 2\gamma d = \ln(100) \Rightarrow d = \frac{\ln 10}{\gamma} = 0.23\ nm$$

Example 17. An electron beam is incident on a potential barrier of height 0.03 eV and of infinite width. Find the reflection coefficient and transmission coefficient at the barrier if the energy of the incident electron beam be (a) 0.04 eV, (b) 0.025 eV.

Soln. (a) In this case, $E > V_0$.

Reflection coefficient $R = \left(\frac{\sqrt{E} - \sqrt{(E-V_0)}}{\sqrt{E} + \sqrt{E-V_0}}\right)^2 \approx 0.1$

Transmission coefficient $T = 1 - R = 1 - 0.1 = 0.9$

(b) In this case, $E < V_0$. So, $T = 0$ and $R = 1$, i.e. all the electrons that are incident on the barrier are reflected back and no electron will be transmitted through the barrier.

3.5 One-Dimensional Rectangular Potential Barrier

Consider a stream of particles each of mass 'm' and energy E be incident from left on the potential barrier surface at $x = 0$, given as following:

$$V(x) = 0 \qquad x < 0$$
$$= V_0 \qquad 0 \le x \le a$$
$$= 0 \qquad x \le a$$

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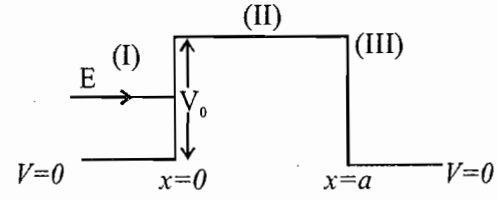

The following two cases arise:

Case 1: If $E > V_0$, then according to classical mechanics the particles will be wholly transmitted and no reflection is possible. But quantum mechanically there is always some probability of reflection at x = 0, back in region I.

Case 2: If $E < V_0$, then classically the particles will be wholly reflected and hence penetration through the barrier is impossible. But quantum mechanically there is always some probability of penetration into the barrier and appearance of the particles in region III. This finite probability of transmission through the barrier even $E<V_0$ is called the quantum mechanical tunnelling effect.

Case A: When $E > V_0$

The time-independent Schrodinger equation for

Region 1: $$-\frac{h^2}{2m}\frac{d^2\psi_1}{dx^2} = E\psi_1 \quad \Rightarrow \quad \frac{d^2\psi_1}{dx^2} + \frac{2mE}{h^2}\psi_1 = 0 \Rightarrow \quad \frac{d^2\psi_1}{dx^2} + \alpha^2\psi_1 = 0 \qquad (28)$$

Region 2: $$-\frac{h^2}{2m}\frac{d^2\psi_2}{dx^2} + V_0\psi_2 = E\psi_2 \Rightarrow \frac{d^2\psi_2}{dx^2} + \frac{2m}{\hbar^2}(E - V_0)\psi_2 = 0 \quad \Rightarrow \quad \frac{d^2\psi_2}{dx^2} + \beta^2\psi_2 = 0 \qquad (29)$$

Region 3: $$-\frac{h^2}{2m}\frac{d^2\psi_3}{dx^2} = E\psi_3 \quad \Rightarrow \quad \frac{d^2\psi_3}{dx^2} + \frac{2mE}{h^2}\psi_3 = 0 \Rightarrow \quad \frac{d^2\psi_3}{dx^2} + \alpha^2\psi_3 = 0 \qquad (30)$$

where, $\alpha^2 = \frac{2mE}{\hbar^2}$ and $\beta^2 = \frac{2m(E - V_0)}{\hbar^2}$.

The general solutions of equations are

$$\psi_1 = Ae^{i\alpha x} + Be^{-i\alpha x}, \quad \psi_2 = Ce^{i\beta x} + De^{-i\beta x}, \quad \psi_3 = Fe^{i\alpha x} + Ge^{-i\alpha x}$$

Since there is no reflected wave in region III, therefore G = 0.

Applying the following boundary conditions:

(i) $(\psi_1)_{x=0} = (\psi_2)_{x=0}$ and (ii) $\left(\frac{d\psi_1}{dx}\right)_{x=0} = \left(\frac{d\psi_2}{dx}\right)_{x=0}$

we will get, $A = \frac{C}{2}\left(1 + \frac{\beta}{\alpha}\right) + \frac{D}{2}\left(1 - \frac{\beta}{\alpha}\right)$ and $B = \frac{C}{2}\left(1 - \frac{\beta}{\alpha}\right) + \frac{D}{2}\left(1 + \frac{\beta}{\alpha}\right)$ (31)

Applying the following boundary conditions:

(i) $(\psi_2)_{x=a} = (\psi_3)_{x=a}$ and (ii) $\left(\frac{d\psi_2}{dx}\right)_{x=a} = \left(\frac{d\psi_3}{dx}\right)_{x=a}$

we will get, $C = \frac{F}{2}\left(1 + \frac{\alpha}{\beta}\right)e^{i(\alpha-\beta)a}$, $D = \frac{F}{2}\left(1 - \frac{\alpha}{\beta}\right)e^{i(\alpha+\beta)a}$ (32)

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Substituting the values of C and D from equation (32) in equation (31) we get,

$$A = \frac{F}{4}e^{i\alpha a}\left[\left(1 + \frac{\beta}{\alpha}\right)\left(1 + \frac{\alpha}{\beta}\right)e^{-i\beta a} + \left(1 - \frac{\beta}{\alpha}\right)\left(1 - \frac{\alpha}{\beta}\right)e^{i\beta a}\right] \qquad (33)$$

$$B = \frac{F}{4}e^{i\alpha a}\left[\left(1 - \frac{\beta}{\alpha}\right)\left(1 + \frac{\alpha}{\beta}\right)e^{-i\beta a} + \left(1 + \frac{\beta}{\alpha}\right)\left(1 - \frac{\alpha}{\beta}\right)e^{i\beta a}\right] \qquad (34)$$

From equation (33), $$\frac{F}{A} = \frac{4e^{-i\alpha a}}{\left(1 + \frac{\beta}{\alpha}\right)\left(1 + \frac{\alpha}{\beta}\right)e^{-i\beta a} + \left(1 - \frac{\beta}{\alpha}\right)\left(1 - \frac{\alpha}{\beta}\right)e^{i\beta a}}$$

$$\Rightarrow \frac{F}{A}=\frac{4\alpha\beta e^{-i\alpha a}}{(\alpha^2+\beta^2)\left(e^{-i\beta a}-e^{i\beta a}\right)+2\alpha\beta\left(e^{-i\beta a}+e^{i\beta a}\right)}=\frac{2\alpha\beta e^{-i\alpha a}}{2\alpha\beta\cos\beta a-i(\alpha^2+\beta^2)\sin\beta a} \quad (35)$$

Reflection and Transmission Coefficients:

Reflection coefficient

$$R=\frac{\text{Reflected flux}\,(J_r)}{\text{Incident flux}\,(J_i)}=\frac{\frac{\hbar\alpha}{m}|B|^2}{\frac{\hbar\alpha}{m}|A|^2}=\frac{|B|^2}{|A|^2}$$

$$\Rightarrow R=\frac{\frac{(\alpha^2-\beta^2)^2}{4\alpha^2\beta^2}\sin^2\beta a}{1+\left(\frac{\alpha^2-\beta^2}{4\alpha^2\beta^2}\right)^2\sin^2\beta a}=\frac{\frac{V_0^2}{4E(E-V_0)}\sin^2\beta a}{1+\frac{V_0^2}{4E(E-V_0)}\sin^2\beta a}$$

Transmission coefficient

$$T=\frac{\text{Transmitted flux}\,(J_t)}{\text{Incident flux}\,(J_i)}=\frac{\frac{\hbar\beta}{m}|F|^2}{\frac{\hbar\alpha}{m}|A|^2}$$

$$\Rightarrow T=\frac{4\alpha^2\beta^2}{4\alpha^2\beta^2\cos^2\beta a+(\alpha^2+\beta^2)^2\sin^2\beta a}=\frac{1}{1+\frac{(\alpha^2-\beta^2)^2}{4\alpha^2\beta^2}\sin^2\beta a}=\frac{1}{1+\frac{V_0^2}{4E(E-V_0)}\sin^2\beta a}$$

Note:

(i) R + T =1

(ii) For $E\to V_0$, $\beta\approx 0\Rightarrow \sin\beta a\approx\beta a$. Therefore,

$$T=\frac{1}{1+\frac{V_0^2}{4E(E-V_0)}(\beta^2a^2)}=\frac{1}{1+\frac{mV_0a^2}{2\hbar^2}}$$

(iii) As E increses above V_0, the increament of $(E-V_0)$ is much more rapid compared to $\sin^2\beta a$, for a fixed width L of the barrier. Therefore, T increases with E.

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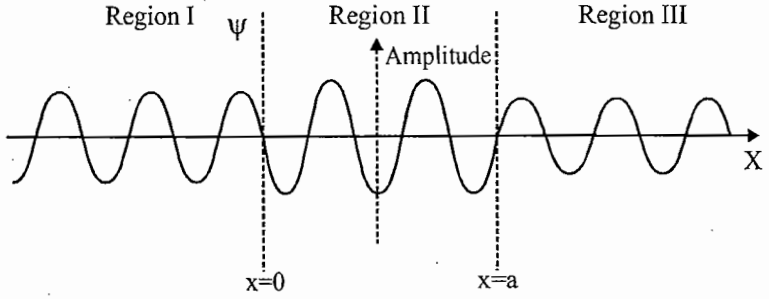
(iv) If the width of the barrier region is an integral multiple of half of the de-Broglie wavelength of the particle in region II, then there will be perfect transmission of the incident beam of particles. This is Ramsauer-Townsend Effect.

(v) For E >> V_0, T = 1 and R = 0.

The natures of the wave functions ψ_1, ψ_2 and ψ_3 in region I, II and III respectively are shown in figure.



Case B : When $E < V_0$

The time-independent Schrodinger equation for

Region 1: $$-\frac{h^2}{2m}\frac{d^2\psi_1}{dx^2} = E\psi_1 \Rightarrow \frac{d^2\psi_1}{dx^2} + \frac{2mE}{h^2}\psi_1 = 0 \Rightarrow \frac{d^2\psi_1}{dx^2} + \alpha^2\psi_1 = 0 \quad (36)$$

Region 2: $$-\frac{h^2}{2m}\frac{d^2\psi_2}{dx^2} + V_0\psi_2 = E\psi_2 \Rightarrow \frac{d^2\psi_2}{dx^2} + \frac{2m}{\hbar^2}(E - V_0)\psi_2 = 0 \Rightarrow \frac{d^2\psi_2}{dx^2} - \beta^2\psi_2 = 0 \quad (37)$$

Region 3: $$-\frac{h^2}{2m}\frac{d^2\psi_3}{dx^2} = E\psi_3 \Rightarrow \frac{d^2\psi_3}{dx^2} + \frac{2mE}{h^2}\psi_3 = 0 \Rightarrow \frac{d^2\psi_3}{dx^2} + \alpha^2\psi_3 = 0 \quad (38)$$

where, $\alpha^2 = \frac{2mE}{\hbar^2}$ and $\beta^2 = \frac{2m(V_0 - E)}{\hbar^2}$.

The general solutions of equations are

$$\psi_1 = Ae^{i\alpha x} + Be^{-i\alpha x}, \quad \psi_2 = Ce^{\beta x} + De^{-\beta x}, \quad \psi_3 = Fe^{i\alpha x} + Ge^{-i\alpha x}$$

Since there is no reflected wave in region III, therefore G = 0.

Applying the following boundary conditions:

(i) $(\psi_1)_{x=0} = (\psi_2)_{x=0}$ and (ii) $\left(\frac{d\psi_1}{dx}\right)_{x=0} = \left(\frac{d\psi_2}{dx}\right)_{x=0}$

we will get, $A = \frac{C}{2}\left(1 + \frac{\beta}{i\alpha}\right) + \frac{D}{2}\left(1 - \frac{\beta}{i\alpha}\right)$ and $B = \frac{C}{2}\left(1 - \frac{\beta}{i\alpha}\right) + \frac{D}{2}\left(1 + \frac{\beta}{i\alpha}\right)$ (39)

Applying the following boundary conditions:

(i) $(\psi_2)_{x=a} = (\psi_3)_{x=a}$ and (ii) $\left(\frac{d\psi_2}{dx}\right)_{x=a} = \left(\frac{d\psi_3}{dx}\right)_{x=a}$

we will get, $C = \frac{F}{2}\left(1 + \frac{i\alpha}{\beta}\right)e^{i\alpha a - \beta a}$, $D = \frac{F}{2}\left(1 - \frac{i\alpha}{\beta}\right)e^{i\alpha a + \beta a}$ (40)

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Substituting the values of C and D from equation (40) in equation (39) we get,

$$A = \frac{F}{4}e^{i\alpha a}\left[\left(1 + \frac{\beta}{i\alpha}\right)\left(1 + \frac{i\alpha}{\beta}\right)e^{-\beta a} + \left(1 - \frac{\beta}{i\alpha}\right)\left(1 - \frac{i\alpha}{\beta}\right)e^{\beta a}\right] \quad (41)$$

$$B = \frac{F}{4}e^{i\alpha a}\left[\left(1 - \frac{\beta}{i\alpha}\right)\left(1 + \frac{i\alpha}{\beta}\right)e^{-\beta a} + \left(1 + \frac{\beta}{i\alpha}\right)\left(1 - \frac{i\alpha}{\beta}\right)e^{\beta a}\right] \quad (42)$$

From equation (43), $$\frac{F}{A} = \frac{4e^{-i\alpha a}}{\left(1 + \frac{\beta}{i\alpha}\right)\left(1 + \frac{i\alpha}{\beta}\right)e^{-\beta a} + \left(1 - \frac{\beta}{i\alpha}\right)\left(1 - \frac{i\alpha}{\beta}\right)e^{\beta a}}$$

$$\frac{F}{A} = \frac{2\alpha\beta e^{-i\alpha a}}{2\alpha\beta\cosh\beta a + i(\beta^2 - \alpha^2)\sinh\beta a}$$

Reflection and Transmission Coefficients:

Reflection coefficient

(36)
$$R = \frac{\text{Reflected flux}\,(J_r)}{\text{Incident flux}\,(J_i)} = \frac{\frac{\hbar\alpha}{m}|B|^2}{\frac{\hbar\alpha}{m}|A|^2} = \frac{|B|^2}{|A|^2}$$

(37)
$$\Rightarrow R = \frac{\frac{(\alpha^2+\beta^2)^2}{4\alpha^2\beta^2}\sinh^2\beta a}{1+\left(\frac{\alpha^2+\beta^2}{4\alpha^2\beta^2}\right)^2\sinh^2\beta a} = \frac{\frac{V_0^2}{4E(V_0-E)}\sinh^2\beta a}{1+\frac{V_0^2}{4E(V_0-E)}\sinh^2\beta a}$$

(38)

Transmission coefficient

$$T = \frac{\text{Transmitted flux}\,(J_t)}{\text{Incident flux}\,(J_i)} = \frac{\frac{\hbar\alpha}{m}|F|^2}{\frac{\hbar\alpha}{m}|A|^2}$$

$$\Rightarrow T = \frac{4\alpha^2\beta^2}{4\alpha^2\beta^2\cosh^2\beta a + (\beta^2-\alpha^2)^2\sinh^2\beta a} = \frac{1}{1+\frac{(\alpha^2+\beta^2)^2}{4\alpha^2\beta^2}\sinh^2\beta a} = \frac{1}{1+\frac{V_0^2}{4E(V_0-E)}\sinh^2\beta a}$$

(39)

Note:

(i) There is a finite probability of transmission of a particle through a potential barrier of width a and height V_0 even if $E < V_0$.

(ii) As E increases, $(V_0 - E)$ decreases and as a result β also decreases. The rate of decrease of $\sin^2\beta a$ for a fixed value of a and V_0 is more than that of $(V_0 - E)$. So T increases steadily with E.

(iii) Again, when $a \to$ large value, $\beta a \to \infty$

(40)
$$\sin h^2(\beta a) = \left(\frac{e^{\beta a} - e^{-\beta a}}{2}\right)^2 = \frac{e^{2\beta a}}{4} = \frac{1}{4}$$

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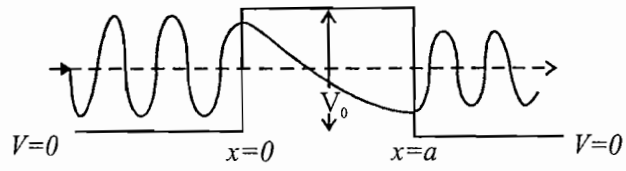
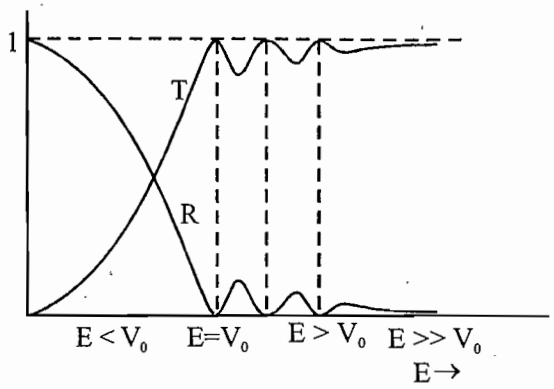
(41)
Therefore, $T = \frac{16E(V_0-E)}{V_0^2}e^{-2\beta a}$

(42)
The natures of the wave functions ψ_1, ψ_2 and ψ_3 in region I, II and III respectively are shown in figure.





Example 20: Calculate the percentage transmission of an electron beam of energy 3eV when incident on a potential barrier of height 4eV and width 20Å.

Soln.: Transmission coefficient $T = \frac{16E}{V_0}\left(1-\frac{E}{V_0}\right)e^{-2\beta a}$

Given: $E = 3eV, V_0 = 4\ eV, a = 20A^0$

Here, $2\beta a = 2a \times \sqrt{\frac{2m}{\hbar^2}(V_0 - E)} \approx 20.49$

Therfore, $T = \frac{16E}{V_0}\left(1-\frac{E}{V_0}\right)e^{-2\beta a} = 3.797 \times 10^{-9}$ (approx)

Hence, the % of transmission is $= 3.797 \times 10^{-9} \times 100 = 3.797 \times 10^{-7}$

Example 21. An alpha particle is trapped in a nucleus of radius 1.4×10^{-15}m. What is the probability that it will escape from the nucleus if its energy is 2MeV? The potential barrier at the surface of the nucleus is 4 MeV and the mass of the α-particle $= 6.64 \times 10^{-27}$ kg

Soln. Transmission coefficient $T = \frac{16E}{V_0}\left(1-\frac{E}{V_0}\right)e^{-2\beta a}$

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Given: $E = 2MeV, V_0 = 4\ MeV, a = 2 \times 1.4 \times 10^{-15} m$

Therefore, transmission co-efficient will be T = 0.124

3.6 One-dimensional linear harmonic oscillator:

If a system vibrates about an equilibrium position such that (a) the magnitude of the force acting on it is proportional to displacement from the equilibrium position, (b) the direction of the force is opposite to that of displacement, then it is called linear harmonic oscillator (LHO).

A simple pendulum, a spring -block system, a floating body etc are familiar examples of a dynamical system that perform simple harmonic motion. In quantum mechanics, linear harmonic oscillator is used in place of simple harmonic oscillator.

Classical Linear Harmonic Oscillator:

Let a time 't', the displacement of particle of mass 'm' constrained to move along the x-axis be x = 0 from equilbirum position. Restoring force on the particle is $F = -kx$ (k is constant).

$$m\frac{d^2x}{dt^2} = -kx \quad \Rightarrow \frac{d^2x}{dt^2} + \omega^2 x = 0 \ \ (\text{where } \omega^2 = \frac{k}{m})$$

The solution of equation (1) can be written as

$$x = a\sin(\omega t + \phi)$$

This represent the simple harmonic motion (SHM) of the particle with frequency,

$$\nu = \frac{\omega}{2\pi} = \frac{1}{2\pi}\sqrt{\frac{k}{m}}$$

Therefore, potential energy of the particle $E_p = \frac{1}{2}kx^2 = \frac{1}{2}m\omega^2 x^2$

and kinetic energy of the particle $E_k = \frac{1}{2}mv^2 = \frac{1}{2}m\omega^2(a^2 - x^2)$

So, total energy of the particle $E = E_p + E_k = \frac{1}{2}m\omega^2 a^2 = \text{constant}$

Quantum Analysis of Linear Harmonic Oscillator:

A particle of mass 'm' is moving under the potential of the form $V = \frac{1}{2}kx^2 = \frac{1}{2}m\omega^2 x^2$

Figure : Schematic diagram of a 1-D linear harmonic oscillator potential.

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Hamiltonian of the system is $H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2$

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Time-independent Schrodinger equation can be written as $\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2\right]\psi = E\psi$ (41)

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}\left[E - \frac{1}{2}m\omega^2 x^2\right]\psi = 0 \quad (42)$$

Solving equation (42), we get the normalized wave function of linear harmonic oscillator in the n^{th} state is

$$\psi_n(x) = \left[\frac{\alpha}{2^n n!\sqrt{\pi}}\right]^{1/2} e^{-\alpha^2 x^2/2} H_n(\alpha x) \quad \text{where, } \alpha^2 = \frac{m\omega}{\hbar} \quad (43)$$

First few wave function of the LHO are as follows:

Ground state (n=0): $\psi_0(x) = \left(\frac{\alpha}{\sqrt{\pi}}\right)^{1/2} e^{-\alpha^2 x^2/2}$

First excited state (n=1): $\psi_1(x) = \left(\frac{\alpha}{2\sqrt{\pi}}\right)^{1/2} (2\alpha x) e^{-\alpha^2 x^2/2}$

Second excited state (n=2): $\psi_2(x) = \left(\frac{\alpha}{8\sqrt{\pi}}\right)^{1/2} (4x^2\alpha^2 - 2) e^{-\alpha^2 x^2/2}$

Third excited state (n=3): $\psi_3(x) = \left(\frac{\alpha}{48\sqrt{\pi}}\right)^{1/2} (8\alpha^3 x^3 - 12\alpha x) e^{-\alpha^2 x^2/2}$

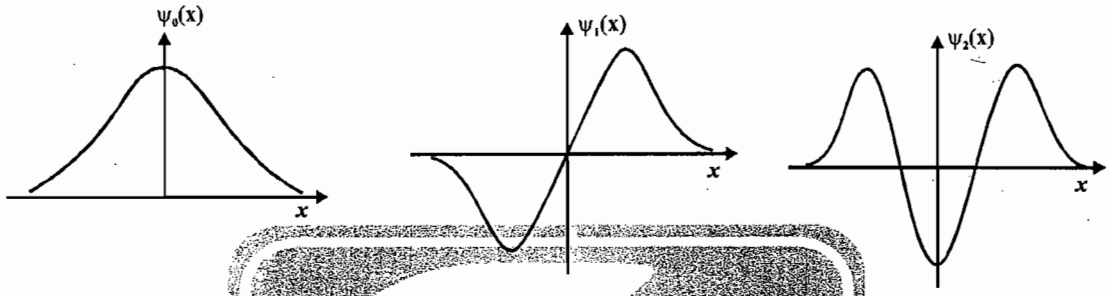

Figure : Schematic diagram of the wavefunction of the particle in ground, first excited and second excited state respectively

Note: (i) $\psi_n(x)$ is an even function if n = even and is an odd function if n = odd.

(ii) $\psi_n(x)$ has 'n' no. of nodes.

Energy eigenvalue of a particle moving under linear harmonic oscillator potential will be

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \qquad [n = 0, 1, 2, 3 \ldots\ldots]$$

It is an infinite sequence of discrete energy levels with equal spacing of $\hbar\omega$. For n = 0, we get $E_0 = \frac{1}{2}\hbar\omega$ and it is known as zero point energy of the oscillator. The existance of zero point energy is in accordance with heisenburg uncertainty principle.

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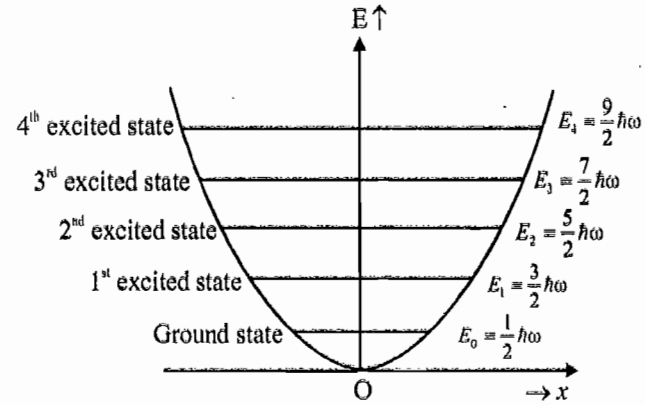

• **Existance of zero point energy according to Uncertainity principle:**

Let a particle of mass 'm' executes SHM along x axis and at time 't' its position is x from the mean position.

Total energy of LHO $E = E_k + E_p = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2 = \frac{(\Delta p)^2}{2m} + \frac{1}{2}m\omega^2(\Delta x)^2$

Since, $\Delta x = x$ then $\Delta p = \frac{\hbar}{2\Delta x} = \frac{\hbar}{2x}$

Therefore, $E = \frac{1}{2m}\left(\frac{\hbar}{2x}\right)^2 + \frac{1}{2}m\omega^2x^2 = \frac{\hbar^2}{8mx^2} + \frac{1}{2}m\omega^2x^2 \Rightarrow \frac{dE}{dx} = -\frac{\hbar^2}{4mx^3} + m\omega^2x$

Putting $\frac{dE}{dx} = 0 \Rightarrow x^2 = \frac{\hbar}{2m\omega}$

Therefore, the miminum energy of the oscillator

$$E_{min} = \frac{\hbar}{8m}\frac{2m\omega}{\hbar} + \frac{1}{2}m\omega^2\frac{\hbar}{2m\omega} = \frac{1}{4}\hbar\omega + \frac{1}{4}\hbar\omega = \frac{1}{2}\hbar\omega$$

Problem 24: A particle of mass 'm' is moving under a potential of the form

$$V(x) = \frac{1}{2}m\omega^2x^2 \qquad x > 0$$
$$= \infty \qquad x \le 0$$

(i) The energy levels are given by

(a) $\left(n+\frac{1}{2}\right)\hbar\omega$ (b) $\left(2n+\frac{1}{2}\right)\hbar\omega$ (c) $\left(2n+\frac{3}{2}\right)\hbar\omega$ (d) $\left(n+\frac{3}{2}\right)\hbar\omega$

(ii) Let the wavefunction of the particle is given by

$$\psi(x) = \frac{1}{\sqrt{5}}\psi_0 + \frac{2}{\sqrt{5}}\psi_1$$

where ψ_0 and ψ_1 are the eigen functions of ground state and first excited state respectively. The expectation value of energy will be

(a) $\frac{31}{10}\hbar\omega$ (b) $\frac{25}{10}\hbar\omega$ (c) $\frac{13}{10}\hbar\omega$ (d) $\frac{11}{10}\hbar\omega$

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Soln. $\psi(x)$ should be zero at $x = 0$

The normalized wavefunction of a particle moving under a linear harmonic oscillator potential is

$$\psi_n(x) = Ae^{-\alpha^2x^2/2}H_n(\alpha x) \quad \left[\text{where } \alpha^2 = \frac{m\omega}{\hbar}\right]$$

$\psi_n(x)$ will be non-zero for n = 0, 2, 4, 6, ... and will be zero for n = 1, 3, 5, 7, ...

So, possible values of 'n' are odd n = 1, 3, 5, 6, ...

(i) The energy eigenvalue of the particle will be

$$E_n = \left(2n+1+\frac{1}{2}\right)\hbar\omega = \left(2n+\frac{3}{2}\right)\hbar\omega \quad (n = 0, 1, 3, ...)$$

(ii) The expectation value of energy will be

$$\langle E\rangle = P_0E_0 + P_1E_1 = \frac{1}{5}\times\frac{3}{2}\hbar\omega + \frac{4}{5}\times\frac{7}{2}\hbar\omega = \frac{31}{10}\hbar\omega$$

Example 25: In a 1-D harmonic Oscillator, two states are defined by

$$\psi_1 = \phi_0 - 2\phi_1 + 3\phi_2$$
$$\psi_2 = \phi_0 - \phi_1 + \alpha\phi_2$$

where ϕ_0, ϕ_1, ϕ_2 are normalized wavefunction corrsespondingh to ground state, first excited state, second state respectively.

(i) The value of α for which ψ_2 is orthogonal to ψ_1 is

(a) 2 (b) 1 (c) –1 (d) –2

(ii) The expectation value of the oscillator in the state ψ_2 is

(a) $\frac{1}{2}\hbar\omega$ (b) $\frac{3}{2}\hbar\omega$ (c) $\frac{5}{2}\hbar\omega$ (d) $\frac{7}{2}\hbar\omega$

Soln. (i) $\langle\psi_2|\psi_1\rangle = 0 \Rightarrow 1+2+3\alpha = 0 \Rightarrow \alpha = -1$

(ii) $\langle E\rangle = \frac{1}{3}\times\frac{1}{2}\hbar\omega + \frac{1}{3}\times\frac{3}{2}\hbar\omega + \frac{1}{3}\times\frac{5}{2}\hbar\omega = \frac{3}{2}\hbar\omega$

Example 27: A particle is initially in the ground state in 1-D harmonic oscillator potential $V(x) = \frac{1}{2}kx^2$. If the spring constant is suddenly doubled, calculate the probability of finding the particle in the ground state of new potential.

Soln. Normalized ground state wave function in old potential will be

$$\psi_0(x) = \left(\frac{\alpha}{\sqrt{\pi}}\right)^{1/2} e^{-\alpha^2x^2/2} \quad \left[\alpha^2 = \frac{m\omega}{\hbar},\ \omega = \sqrt{\frac{k}{m}}\right]$$

Normalized ground state wave function in new potential will be

$$\psi'_0(x) = \left(\frac{\alpha'}{\sqrt{\pi}}\right)^{1/2} e^{-\alpha'^2x^2/2} \quad \left[\alpha'^2 = m\omega'/\hbar,\ \omega' = \sqrt{\frac{2k}{m}}\right]$$

Required probability $P = |\langle\psi'_0|\psi_0\rangle|^2$

$$|\langle\psi'_0|\psi_0\rangle| = \int_{-\infty}^{\infty}\left(\frac{\alpha\alpha'}{\pi}\right)^{1/2} e^{-(\alpha^2+\alpha'^2)x^2/2}dx = \sqrt{\frac{2\alpha\alpha'}{(\alpha^2+\alpha'^2)}}$$

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$$P = \frac{2\alpha\alpha'}{\alpha^2+\alpha'^2} = \frac{2\times\sqrt{\frac{m\omega}{\hbar}}\sqrt{\frac{m\omega'}{\hbar}}}{\frac{m\omega}{\hbar}+\frac{m\omega'}{\hbar}} = \frac{2\times\frac{m\omega}{\hbar}\left(\sqrt{2}\right)^{1/2}}{\frac{m\omega}{\hbar}\left(1+\sqrt{2}\right)} = \frac{2^{5/4}}{1+\sqrt{2}}$$

Operator formalism of harmonic Oscillator:

Hamiltonian of the system is $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2$

Defining two dimensionless operators

$$\hat{P} = \frac{\hat{p}}{\sqrt{m\hbar\omega}} \text{ and } \hat{X} = \hat{x}\sqrt{\frac{m\omega}{\hbar}}$$

The hamiltonian can be written as, $\hat{H}=\frac{\hbar\omega}{2}\left[\frac{\hat{p}^2}{m\hbar\omega}+\frac{m\omega}{2\hbar}\hat{x}^2\right]=\frac{\hbar\omega}{2}\left[\hat{P}^2+\hat{X}^2\right]$

Introducing two non-hermitian operators, $\hat{a}=\frac{1}{\sqrt{2}}\left[\hat{X}+i\hat{P}\right]$, $\hat{a}^\dagger=\frac{1}{\sqrt{2}}\left[\hat{X}-i\hat{P}\right]$

where $\hat{a}$ and $\hat{a}^\dagger$ are hermitian conjugate to each other.

Now, $\hat{a}^\dagger\hat{a}=\frac{1}{2}\left[\hat{X}^2+\hat{P}^2+i\hat{X}\hat{P}-i\hat{P}\hat{X}\right]=\frac{1}{2}\left(\hat{P}^2+\hat{X}^2\right)+\frac{i}{2}\left[\hat{X},\hat{P}\right]$

$\Rightarrow\hat{a}^\dagger\hat{a}=\frac{\hat{H}}{\hbar\omega}-\frac{1}{2}\Rightarrow\hat{H}=\left(\hat{a}^\dagger\hat{a}+\frac{1}{2}\right)\hbar\omega\ \Rightarrow\hat{H}=\left(\hat{N}+\frac{1}{2}\right)\hbar\omega$

where, $\hat{N}=\hat{a}^\dagger\hat{a}$ = number operator/occupation number operator.

- **Some important commutation relations:**

(i) $\left[\hat{a},\hat{a}^\dagger\right]=1$ (ii) $\left[\hat{a}^\dagger\hat{a},\hat{a}^\dagger\right]=\hat{a}^\dagger$ (iii) $\left[\hat{a}^\dagger\hat{a},\hat{a}\right]=-\hat{a}$

(iv) $\left[\hat{H},\hat{a}^\dagger\hat{a}\right]=0$ (v) $\left[\hat{a},\hat{H}\right]=\hbar\omega\hat{a}$ (vi) $\left[\hat{a}^\dagger,\hat{H}\right]=-\hbar\omega\hat{a}^\dagger$

- **Lowering operator and Raising operator:**

$\hat{H}\left(\hat{a}|n\rangle\right)=\left(\hat{a}\hat{H}-\hbar\omega\hat{a}\right)|n\rangle=\hat{a}E_n|n\rangle-\hbar\omega\hat{a}|n\rangle=\left(E_n-\hbar\omega\right)\left(\hat{a}|n\rangle\right)$

So, that, $\hat{a}|n\rangle$ is the eigenstates of $\hat{H}$ operator corresponding eigenvalue $\left(E_n-\hbar\omega\right)$. Action of $\hat{a}$ on $|n\rangle$ generate new energy states that is lower by one unit energy $\hbar\omega$ i.e.

$\hat{a}|n\rangle=C_n|n-1\rangle\ \Rightarrow\langle n|\hat{a}^\dagger=\langle n-1|c_n^*$

Therefore, $\langle n|\hat{a}^\dagger\hat{a}|n\rangle=\langle n-1|n-1\rangle|c_n|^2\Rightarrow n=|c_n|^2\Rightarrow|c_n|=\sqrt{n}$

So, $\hat{a}|n\rangle=\sqrt{n}|n-1\rangle$

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Similarly, $\hat{H}\left(\hat{a}^\dagger|n\rangle\right)=\left(\hat{a}^\dagger\hat{H}+\hbar\omega\hat{a}^\dagger\right)|n\rangle=\left(E_n+\hbar\omega\right)\left(\hat{a}^\dagger|n\rangle\right)$

So, that, $\hat{a}^\dagger|n\rangle$ are the eigenstates of $\hat{H}$ operator corresponding eigenvalue $\left(E_n+\hbar\omega\right)$. Action of $\hat{a}^\dagger$ on $|n\rangle$ generate new energy states that is higher by one unit energy $\hbar\omega$.

$$\hat{a}^\dagger|n\rangle=c_n|n+1\rangle\ \Rightarrow\langle n|\hat{a}=\langle n+1|c_n^*$$

Therefore, $\langle n|\hat{a}\hat{a}^\dagger|n\rangle=|c_n|^2\langle n+1|n+1\rangle\Rightarrow(n+1)=|c_n|^2\Rightarrow|c_n|=\sqrt{n+1}$

So, $$\hat{a}^\dagger|n\rangle=\sqrt{n+1}|n+1\rangle$$

Therefore, the nth state can be written in terms of ground state as

$$|n\rangle=\frac{\left(\hat{a}^\dagger\right)^n}{\quad}|0\rangle$$

Calculation of normalized wave function:

Ground state wavefunction:

Since, action of $\hat{a}$ on $|n\rangle$ generate new energy states that is lower by one unit energy $\hbar\omega$, then

$$\hat{a}|0\rangle = 0$$

$$\Rightarrow \left\{\sqrt{\frac{m\omega}{2\hbar}}\hat{x} + i\frac{\hat{p}}{\sqrt{2m\omega\hbar}}\right\}\psi_0 = 0 \Rightarrow \sqrt{\frac{m\omega}{2\hbar}}x\psi_0 + \frac{\hbar}{\sqrt{2m\omega\hbar}}\psi_0 = 0$$

$$\Rightarrow \frac{d\psi_0}{dx} = -\frac{m\omega}{\hbar}x\psi_0 \Rightarrow \frac{d\psi_0}{\psi_0} = -\frac{m\omega}{\hbar}xdx \Rightarrow \ell n\psi_0 = -\frac{m\omega}{\hbar}\frac{x^2}{2} + \ell nA$$

$$\Rightarrow \psi_0(x) = A\exp\left(-\frac{m\omega}{\hbar}\frac{x^2}{2}\right) \Rightarrow \psi_0(x) = A\exp\left(-\frac{\alpha^2x^2}{2}\right) \text{ [where } \alpha^2 = \frac{m\omega}{\hbar}\text{]}$$

Normalization Condition: $\int_{-\infty}^{\infty}\psi_0^*(x)\psi_0(x)dx = 1$

$$\Rightarrow 2|A|^2\int_0^{\infty}\exp\left(-\alpha^2x^2\right)dx = 1 \Rightarrow A = \left(\frac{\alpha}{\sqrt{\pi}}\right)^{1/2}$$

Therefore, normalized ground state wavefunction will be

$$\psi_0(x) = \left(\frac{\alpha}{\sqrt{\pi}}\right)^{1/2}e^{-\alpha^2x^2/2}$$

First excited state wavefunction:

Since, $\hat{a}^{\dagger}|0\rangle = |1\rangle$

$$\Rightarrow \quad |1\rangle = \left[\sqrt{\frac{m\omega}{2\hbar}}\hat{x} - \frac{i}{\sqrt{2m\omega\hbar}}\hat{p}\right]|0\rangle$$

$$= \left[\sqrt{\frac{m\omega}{2\hbar}}\hat{x} - \frac{i}{\sqrt{2m\omega\hbar}}\left(i\hbar\frac{\partial}{\partial x}\right)\right]|0\rangle$$

$$= \sqrt{\frac{m\omega}{2\hbar}}x\left[\frac{\alpha}{\sqrt{\pi}}\right]^{1/2}e^{-\frac{\alpha^2x^2}{2}} - \frac{\hbar}{\sqrt{2m\omega\hbar}}\left[\frac{\alpha}{\sqrt{\pi}}\right]^{1/2}e^{-\alpha^2x^2/2}\left(-\alpha^2x\right)$$

$$= \left[\frac{\alpha}{\sqrt{4}.\sqrt{\pi}}\right]^{1/2}e^{\frac{-\alpha^2x^2}{2}}(2\alpha x) = \left[\frac{\alpha}{2\sqrt{\pi}}\right]^{1/2}e^{\frac{-\alpha^2x^2}{2}}H_1(\alpha x)$$

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Expectation value of a odd operator for a symmetric potential:

The wave function of a particle is moving under a symmetric potential $V(-x) = V(x)$, has a definite parity i.e it will be of either even or odd parity.

Therefore, expectation value of an odd operator $= \langle\hat{A}\rangle = \langle\psi|\hat{A}|\psi\rangle = 0$

Similarly, $\langle\hat{A}^m\rangle = \langle\psi|\hat{A}^m|\psi\rangle = 0$ (m = odd integer)

Calculation of expectation value using operator formalism:

As we know, $\hat{a}=\sqrt{\frac{m\omega}{2\hbar}}\hat{x}+\hat{p}\frac{i}{\sqrt{2m\omega\hbar}}$ and $\hat{a}^{\dagger}=\sqrt{\frac{m\omega}{2\hbar}}\hat{x}-\hat{p}\frac{i}{\sqrt{2m\omega\hbar}}$,

therefore we get,

$$\hat{x}=\sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a}+\hat{a}^{\dagger}\right) \text{ and } \qquad \hat{p}=\frac{1}{i}\sqrt{\frac{\hbar m\omega}{2}}\left(\hat{a}-\hat{a}^{\dagger}\right)$$

$$\langle\hat{x}\rangle=\sqrt{\frac{\hbar}{2m\omega}}\left\langle n\left|\left(\hat{a}+\hat{a}^{\dagger}\right)\right|n\right\rangle=\sqrt{\frac{\hbar}{2m\omega}}\left[\sqrt{n}\langle n|n-1\rangle+\sqrt{n+1}\langle n|n+1\rangle\right]=0$$

$$\langle\hat{p}\rangle=\frac{1}{i}\sqrt{\frac{\hbar m\omega}{2}}\left\langle n\left|\hat{a}-\hat{a}^{\dagger}\right|n\right\rangle=\frac{1}{i}\sqrt{\frac{\hbar m\omega}{2}}\left[\sqrt{n}\langle n|n-1\rangle-\sqrt{n+1}\langle n|n+1\rangle\right]=0$$

$$\left\langle\hat{x}^2\right\rangle=\frac{\hbar}{2m\omega}\left\langle n\left|\left(\hat{a}+\hat{a}^{\dagger}\right)\left(\hat{a}^{\dagger}+\hat{a}\right)\right|n\right\rangle=\frac{\hbar}{2m\omega}\left\langle n\left|\left(\hat{a}^2+\hat{a}^{\dagger^2}+\hat{a}\hat{a}^{\dagger}+\hat{a}^{\dagger}\hat{a}\right)\right|n\right\rangle$$

$$=\frac{\hbar}{2m\omega}\left[\sqrt{n}\sqrt{n-1}\langle n|n-2\rangle+\sqrt{n+1}\sqrt{n+2}\langle n|n+1\rangle+\sqrt{n+1}\sqrt{n+1}\langle n|n\rangle+\sqrt{n}\sqrt{n}\langle n|n\rangle\right]$$

$$=\frac{\hbar}{2m\omega}(2n+1)=\frac{\hbar}{m\omega}\left(n+\frac{1}{2}\right)$$

Similarly, $\left\langle p^2\right\rangle=\left(n+\frac{1}{2}\right)m\hbar\omega$

Uncertainity in position $\Delta x=\sqrt{\left\langle x^2\right\rangle-\langle x\rangle^2}=\sqrt{\frac{\hbar}{m\omega}\left(n+\frac{1}{2}\right)}$

Uncertainity in momentum $\Delta p=\sqrt{\left\langle p^2\right\rangle-\langle p\rangle^2}=\sqrt{\left(n+\frac{1}{2}\right)\hbar m\omega}$

Therefore, the uncertainity product becomes $\Delta x\Delta p=\left(n+\frac{1}{2}\right)\hbar$

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Example 26: Let $|0\rangle$ and $|1\rangle$ denote the normalized eigenstates corresponding to the ground and first state of a 1-D harmonic oscillator. The uncertainty Δp in the state $\frac{1}{\sqrt{2}}(|0\rangle+|1\rangle)$ is:

(a) $\frac{\sqrt{m\omega\hbar}}{2}$ (b) $\sqrt{\frac{m\omega\hbar}{2}}$ (c) $\sqrt{m\omega\hbar}$ (d) $\sqrt{2m\omega\hbar}$

Soln. $\langle\hat{p}\rangle=\frac{1}{2}\left[\langle 0|\hat{p}|0\rangle+\langle 0|\hat{p}|1\rangle+\langle 1|\hat{p}|0\rangle+\langle 1|\hat{p}|1\rangle\right]=\frac{1}{2}\left[0+\frac{1}{i}\sqrt{\frac{m\omega\hbar}{2}}-\frac{1}{i}\sqrt{\frac{m\omega\hbar}{2}}+0\right]=0$

$$\left\langle\hat{p}^2\right\rangle=\frac{1}{2}\left[\left\langle 0\left|\hat{p}^2\right|0\right\rangle+\left\langle 0\left|\hat{p}^2\right|1\right\rangle+\left\langle 1\left|\hat{p}^2\right|0\right\rangle+\left\langle 1\left|\hat{p}^2\right|1\right\rangle\right]=\frac{1}{2}\left[m\hbar\omega\frac{1}{2}+0+0+\frac{3}{2}m\hbar\omega\right]=m\omega\hbar$$

Uncertainity in the momentum in the given state will be

$$\Delta p=\sqrt{\left\langle p^2\right\rangle-\langle p\rangle^2}=\sqrt{\hbar m\omega}$$

Example 27: The wave function of a linear harmonic oscillator in the potential $V(x)=\frac{1}{2}m\omega^2x^2$ at a given instant is $\psi(x)=\left(\frac{2}{\pi\beta^2}\right)^{1/4}e^{-x^2/\beta^2}$. For what value of β will the function $a\psi(x)$ be zero?

Soln. $a=\frac{1}{\sqrt{2}}\left(\hat{X}+i\hat{P}_x\right)=\frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega}{\hbar}}x+i\frac{p_x}{\sqrt{m\hbar\omega}}\right)=\frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega}{\hbar}}x+\sqrt{\frac{\hbar}{m\omega}}\frac{d}{dx}\right)$

Thus, $a\psi(x)=\frac{1}{\sqrt{2}}\left(\frac{2}{\pi\beta^2}\right)^{1/4}\left(\sqrt{\frac{m\omega}{\hbar}}x+\sqrt{\frac{\hbar}{m\omega}}\frac{d}{dx}\right)e^{-x^2/\beta^2}$

$=\left(\frac{1}{2\pi\beta^2}\right)^{1/4}\left(\sqrt{\frac{m\omega}{\hbar}}x+\sqrt{\frac{\hbar}{m\omega}}\left(-\frac{2x}{\beta^2}\right)\right)e^{-x^2/\beta^2}$

$=\left(\frac{1}{2\pi\beta^2}\right)^{1/4}\left(\sqrt{\frac{m\omega}{\hbar}}-\frac{2}{\beta^2}\sqrt{\frac{\hbar}{m\omega}}\right)xe^{-x^2/\beta^2}$

This will be zero if $\beta=\sqrt{\frac{2\hbar}{m\omega}}$.

Example 28. Consider a particle of mass 'm' and charge 'q' placed in a uniform electric field $E=E_0\hat{i}$. Apart from the force due to the electric field, a restoring force corresponding to the potential $V_1(x)=\frac{1}{2}m\omega^2x^2$ acts on the particle. Find the energy eigenvalues of the particle, taking the electric potential energy to be zero at the origin.

Soln. The electric potential enregy at the position 'x' will be $-qE_0x$. Thus, the net potential is

$$V(x)=\frac{1}{2}m\omega^2x^2-qE_0x=\frac{1}{2}m\omega^2\left(x^2-\frac{2qE_0}{m\omega^2}x\right)$$

$$=\frac{1}{2}m\omega^2\left(x-\frac{qE_0}{m\omega^2}\right)^2-\frac{q^2E_0^2}{2m\omega^2}$$

If you shift the origin of 'x' to $\frac{qE_0}{m\omega^2}$ and define $x'=\left(x-\frac{qE_0}{m\omega^2}\right)$, the potential as a function of x' is

$$V(x')=\frac{1}{2}m\omega^2x'^2-\frac{q^2E_0^2}{2m\omega^2}$$

This is the potential of a linear harmonic oscillator with energy $-\frac{q^2E_0^2}{2m\omega^2}$ at $x'=0$. This is a constant shift in the energy eigenvalues are $\left(n+\frac{1}{2}\right)\hbar\omega-\frac{q^2E_0^2}{2m\omega^2}$.

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Example 29. A linear harmonic oscillator is in its ground state. Find the range of 'x' that is allowed classically. Calculate the probability of finding it in the classically forbidden region.

Soln. For classically allowed region, the total energy E should be greater than or equal to the potential energy. For linear harmonic oscillator in ground state, this region is given by

$$\frac{\hbar\omega}{2} \geq \frac{1}{2}m\omega^2x^2 \Rightarrow x^2 \leq \frac{\hbar}{m\omega} \Rightarrow -\sqrt{\frac{\hbar}{m\omega}} \leq x \sqrt{\frac{\hbar}{m\omega}}$$

The probability of finding the oscillator in this range is

$$\int_{-\sqrt{\hbar/m\omega}}^{\sqrt{\hbar/m\omega}} \left|\psi_0(x)^2\right|^2 dx = 2 \times \int_0^{\sqrt{\hbar/m\omega}} \sqrt{\frac{m\omega}{\pi\hbar}} e^{-\left(\frac{m\omega}{\hbar}\right)x^2} dx$$

Assuming, $t = \sqrt{\frac{m\omega}{\hbar}}x$, the above expression becomes $2\sqrt{\frac{m\omega}{\pi\hbar}}\sqrt{\frac{\hbar}{m\omega}}\int_0^1 e^{-t^2}dt \approx 0.84$

Thus the probability of finding the oscillator in the classically forbidden region is 1–0.84 = 0.16.

Example 30. A particle of mass 'm' moves in the potential $V(x) = \frac{1}{2}m\omega^2x^2$. It has wave function $\psi(x)$ at time t = 0. What will be the wave function at $t = \frac{2\pi}{\omega}$ (one time period)?

Soln. Let the wave function at $t = 0$ be $\psi(x) = \sum_n C_n|\phi_n\rangle$

The wave function at time t will be

$$\psi(x,t) = \sum_n C_n|\phi_n\rangle e^{-\frac{i}{\hbar}E_nt} = \sum_n C_n|\phi_n\rangle e^{-\frac{i}{\hbar}\left(n+\frac{1}{2}\right)\hbar\omega t}$$

$$= \sum_n C_n|\phi_n\rangle e^{-\left(n+\frac{1}{2}\right)2\pi} = \sum_n C_n|\phi_n\rangle e^{-i\pi} = -\sum_n C_n|\phi_n\rangle = -\psi(x)$$

In one time period the wave function becomes negative of its original form. In two time periods, it regains its original shape.

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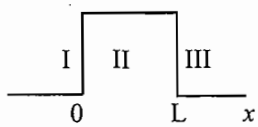
Example 31. A particle of mass 'm' is incident on a rectangular potential barrier of height V_0 extended from $x = 0$ to $x = L$. The energy of the particle is $E = V_0 + \frac{\hbar^2\pi^2}{2mL^2}$. Write the wave function in the three regions and by using the boundary conditions show that there is no reflected wave.

Soln. The general form of the wave function is

$$\psi_I = A_1 e^{ik_1x} + B_1e^{-ik_1x}$$

$$\psi_{II} = A_2 e^{ik_2x} + B_2e^{-ik_2x}$$

$$\psi_{III} = A_3 e^{ik_1x}$$



where, $k_2 = \sqrt{\frac{2m(E-V_0)}{\hbar^2}} = \frac{\pi}{L}$; $k_1 = \sqrt{\frac{2mE}{\hbar^2}}$

Boundary conditions at $x = 0$,

$$\psi_I(x) = \psi_{II}(0) \quad \Rightarrow A_1 + B_1 = A_2 + B_2 \quad \text{... (i)}$$

$$\left.\frac{d\psi_I}{dx}\right|_0 = \left.\frac{d\psi_{II}}{dx}\right|_0 \quad \Rightarrow \quad k_1(A_1 - B_1) = k_2(A_2 - B_2) \quad \text{... (ii)}$$

Boundary conditions at $x = L$,

$$\psi_{II}(L) = \psi_{III}(L) \quad \Rightarrow \quad A_2 e^{ik_2 L} + B_2 e^{-ik_2 L} = A_3 e^{ik_1 L} \quad \text{... (iii)}$$

$$\left.\frac{d\psi_{II}}{dx}\right|_L = \left.\frac{d\psi_{III}}{dx}\right|_L \quad \Rightarrow ik_2\left(A_2 e^{ik_2 L} - B_2 e^{-ik_2 L}\right) = ik_1 A_3 e^{ik_1 L} \quad \text{... (iv)}$$

According to the question, $e^{ik_2 L} = e^{i\pi} = -1$ and $e^{-ik_2 L} = e^{-i\pi} = -1$

So, (iii) and (iv) becomes

$$-(A_2 + B_2) = A_3 e^{ik_1 L}$$

$$-k_2(A_2 - B_2) = k_1 A_3 e^{ik_1 L}$$

But from (i) and (ii) $\dfrac{A_2 + B_2}{A_2 - B_2} = \dfrac{k_2}{k_1}\dfrac{A_1 + B_1}{A_1 - B_1}$

Thus, $\dfrac{k_2}{k_1} = \dfrac{k_2}{k_1}\dfrac{A_1 + B_1}{A_1 - B_1} \Rightarrow A_1 + B_1 = A_1 - B_1 \Rightarrow B_1 = 0$

Hence, there is no reflected wave.

Example 32. A linear harmonic oscillator is in the first excited state. (i) At what point is its probability density maximum? (ii) What is the value of maximum probability density?

Soln. The harmonic oscillator wave function in the $n = 1$ state is

$$\psi_1(x) = \left(\frac{\alpha}{2\sqrt{\pi}}\right)^{1/2} 2\alpha x \exp\left(\frac{-\alpha^2 x^2}{2}\right), \text{ where } \alpha = \left(\frac{m\omega}{\hbar}\right)^{1/2}$$

(i) Probability density $P(x) = \psi\psi^* = \dfrac{2\alpha^3}{\sqrt{\pi}} x^2 \exp(-\alpha^2 x^2)$

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$P(x)$ is maximum when $dP/dx = 0 \Rightarrow \dfrac{2\alpha^3}{\sqrt{\pi}}(2x - 2\alpha^2 x^3) = 0 \Rightarrow x = \pm\dfrac{1}{\alpha}$

(ii) Maximum value of $P(x) = \dfrac{2\alpha}{\sqrt{\pi}}\dfrac{1}{e} = \dfrac{2\alpha}{\sqrt{\pi}}\dfrac{1}{2.718} = 0.415\alpha$

Example 33. Consider a particle of mass m in the one-dimensional short range potential $V(x) = -V_0\delta(x)$, $V_0 > 0$ where $\delta(x)$ is the Dirac delta function. Find the energy of the system.

Soln. The Schrodinger equation for such a potential is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} - V_0\delta(x)\psi(x) = E\psi(x)$$

$$\Rightarrow \frac{d^2\psi}{dx^2} + \frac{2mE\psi}{\hbar^2} = -\frac{2mV_0}{\hbar^2}\delta(x)\psi$$

Since the potential is attractive, then $E < 0$ for bound states

$$\frac{d^2\psi}{dx^2} - k^2\psi = -\frac{2mV_0}{\hbar^2}\delta(x)\psi\,, \quad k^2 = -\frac{2mE}{\hbar^2} \tag{1}$$

For all points except at $x = 0$, the equation becomes $\frac{d^2\psi}{dx^2} - k^2\psi = 0$

Soloution of the above equation, will be

$$\psi(x) = \begin{cases} e^{-kx}, & x > 0 \\ e^{kx}, & x > 0 \end{cases} \tag{2}$$

(the solution must vanish at $x \to \pm\infty$)

The normalization factor is assumed to be unity.

Integrating equation (1) from $-\lambda$ to $+\lambda, \lambda$ being an arbitrarily small positive number, we get

$$\left(\frac{d\psi}{dx}\right)_{-\lambda}^{\lambda} - k^2\int_{-\lambda}^{\lambda}\psi dx = -\frac{2mV_0}{\hbar^2}\int_{-\lambda}^{\lambda}\delta(x)\psi(x)dx$$

In the limit $\lambda \to 0$, the above equation becomes

$$\left(\frac{d\psi}{dx}\right)_{x=0+} - \left(\frac{d\psi}{dx}\right)_{x=0-} = -\frac{2mV_0}{\hbar^2}\psi(0)$$

$$\Rightarrow -k\psi(0) - k\psi(0) = -\frac{2mV_0}{\hbar^2}\psi(0)$$

$$\Rightarrow k = \frac{mV_0}{\hbar^2} \Rightarrow \frac{2mE}{\hbar^2} = \frac{mV_0}{\hbar^2} \Rightarrow E = -\frac{mV_0^2}{2\hbar^2}$$

Example 35. Consider two identical linear oscillators having a spring constant k. The interaction potential is $H = Ax_1x_2$ where x_1 and x_2 are the coordinates of the oscillators. Obtain the energy eigenvalues.

Soln. The Hamiltonian of the system is

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_1^2} - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_2^2} + \frac{1}{2}m\omega^2x_1^2 + \frac{1}{2}m\omega^2x_2^2 + Ax_1x_2$$

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Substituting $x_1 = \frac{1}{\sqrt{2}}(y_1 + y_2), \quad x_2 = \frac{1}{\sqrt{2}}(y_1 - y_2)$

We can have $H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y_1^2} - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial y_2^2} + \frac{1}{2}m\omega^2(y_1^2 + y_2^2) + \frac{A}{2}(y_1^2 - y_2^2)$

$$= -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y_1^2} - \frac{1}{2}m\left(\omega^2 + \frac{A}{m}\right)y_1^2 - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial y_2^2} + \frac{1}{2}m\left(\omega^2 - \frac{A}{m}\right)y_2^2$$

Hence the system can be regarded as two independent harmonic oscillators having coordinates y_1 and y_2. The energy levels are

$$E_{nn'} = \left(n + \frac{1}{2}\right)\hbar\sqrt{\left(\omega^2 + \frac{A}{m}\right)} + \left(n' + \frac{1}{2}\right)\hbar\sqrt{\left(\omega^2 - \frac{A}{m}\right)}$$

CSIR PREVIOUS YEAR QUESTIONS

1. The wavefunction of a particle is given by $\psi = \left(\frac{1}{\sqrt{2}}\phi_0 + i\phi_1\right)$, where ϕ_0 and ϕ_1 are the normalized eigenfinctions with energies E_0 and E_1 corresponding to the ground state and first excited state, respectively. The expectation value of the Hamiltonian in the state ψ is: **[CSIR June -2011]**

(a) $\frac{E_0}{2} + E_1$ (b) $\frac{E_0}{2} - E_1$ (c) $\frac{E_0 - 2E_1}{3}$ (d) $\frac{E_0 + 2E_1}{3}$

Soln. Normalization of ψ :

$$|\psi\rangle = A\left[\frac{1}{\sqrt{2}}|\phi_0\rangle + i|\phi_1\rangle\right]$$

Applying normalization condition i.e. $\langle\psi|\psi\rangle = 1 \quad \Rightarrow \frac{A^2}{2} + A^2 = 1 \quad \Rightarrow A = \sqrt{\frac{2}{3}}$

So, normalized wavefunctton of the particle $|\psi\rangle = \frac{1}{\sqrt{3}}|\phi_0\rangle + i\sqrt{\frac{2}{3}}|\phi_1\rangle$

Expexted value of the Hamiltonian in the state $|\psi\rangle$ i.e.

$$\langle H\rangle = P_0E_0 + P_1E_1 = |c_0|^2E_0 + |c_1|^2E_1 = \frac{1}{3}E_0 + \frac{2}{3}E_1 = \frac{E_0 + 2E_1}{3}$$

Correct option is (d)

2. A particle is confined to the region $x \geq 0$ by a potential which increases linearly as $u(x) = u_0x$. The mean position of the particle at temperature T is: **[CSIR June -2011]**

(a) $\frac{k_BT}{u_0}$ (b) $(k_BT)^2/u_0$ (c) $\sqrt{\frac{k_BT}{u_0}}$ (d) u_0k_BT

Soln. According to virial Theorem, if potential $u(x) \propto x^n$, then $\langle\text{Kinetic energy}\rangle = \frac{n}{2}\langle\text{Potential energy}\rangle$

For given potential $u(x) = u_0x$, $\langle\text{Kinetic energy}\rangle = \frac{1}{2}\langle\text{Potential energy}\rangle$

According to equipartition Theorem,

$$\langle\text{Energy}\rangle = \frac{3}{2}k_BT \Rightarrow \langle\text{K.E.}\rangle + \langle\text{P.E.}\rangle = \frac{3}{2}k_BT \Rightarrow \frac{3}{2}\langle\text{P.E.}\rangle = \frac{3}{2}k_BT$$

$$\Rightarrow u_0\langle x\rangle = k_BT \quad \Rightarrow \langle x\rangle = \frac{k_BT}{u_0}$$

Correct option is (a)

3. Consider a praticle in a one dimensional potential that satisfies $V(x) = V(-x)$. Let $|\psi_0\rangle$ and $|\psi_1\rangle$ denote the ground and the first excited states, respectively, and let $|\psi\rangle = \alpha_0|\psi_0\rangle + \alpha_1|\psi_1\rangle$ be a normalized state with α_0 and α_1 being real constants. The expectation value $\langle x\rangle$ of the position operator x in the state $|\psi\rangle$ is given by **[CSIR Dec 2011]**

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(a) $\alpha_0^2\langle\psi_0|x|\psi_0\rangle+\alpha_1^2\langle\psi_1|x|\psi_1\rangle$ (b) $\alpha_0\alpha_1\left[\langle\psi_0|x|\psi_1\rangle+\langle\psi_1|x|\psi_0\rangle\right]$

(c) $\alpha_0^2+\alpha_1^2$ (d) $2\alpha_0\alpha_1$

Soln. $\langle x\rangle=\dfrac{\langle\psi|x|\psi\rangle}{\langle\psi|\psi\rangle}$ $=\left(\langle\psi_0|\alpha_0+\langle\psi_1|\alpha_1\right)x\left(\alpha_0|\psi_0\rangle+\alpha_1|\psi_1\rangle\right)$

$=\alpha_0^2\langle\psi_0|x|\psi_0\rangle+\alpha_1^2\langle\psi_1|x|\psi_1\rangle+\alpha_0\alpha_1\langle\psi_0|x|\psi_1\rangle+\alpha_0\alpha_1\langle\psi_1|x|\psi_0\rangle$

For a particle moving under a symmetric potential, the wavefunction will have definte parity i.e. either even or odd. Therefore, the first and second term will be zero as the corresponding integral will be odd in nature. So,

$$\langle x\rangle=\alpha_0\alpha_1\left[\langle\psi_0|x|\psi_1\rangle+\langle\psi_1|x|\psi_0\rangle\right]$$

Correct option is (b)

4. Let $|0\rangle$ and $|1\rangle$ denote the normalized eigenstates corresponding to the ground and first excited state of a one dimensional harmonic oscillator. The uncertainty Δp in the state $\frac{1}{\sqrt{2}}\left(|0\rangle+|1\rangle\right)$, is:

[CSIR Dec 2011]

(a) $\Delta p=\sqrt{\hbar m\omega}/2$ (b) $\Delta p=\sqrt{\hbar m\omega}/2$

(c) $\Delta p=\sqrt{\hbar m\omega}$ (d) $\Delta p=\sqrt{2\hbar m\omega}$

Soln. $\langle p\rangle=\langle\psi|\hat{p}|\psi\rangle=\dfrac{1}{2}\left[\langle 0|\hat{p}|0\rangle+\langle 1|\hat{p}|1\rangle+\langle 0|\hat{p}|1\rangle+\langle 1|\hat{p}|0\rangle\right]$

$=-i\sqrt{\dfrac{\hbar m\omega}{2}}\times\dfrac{1}{2}\left[\langle 0|\left(\hat{a}-\hat{a}^\dagger\right)|0\rangle+\langle 1|\left(\hat{a}-\hat{a}^\dagger\right)|1\rangle+\langle 0|\left(\hat{a}-\hat{a}^\dagger\right)|1\rangle+\langle 1|\left(\hat{a}-\hat{a}^\dagger\right)|0\rangle\right]$

$=-\dfrac{i}{2}\sqrt{\dfrac{\hbar m\omega}{2}}[0+0+1-1]=0$

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$\hat{p}^2=\left(-i\sqrt{\dfrac{\hbar m\omega}{2}}\right)^2\left[\hat{a}^2+\hat{a}^{\dagger 2}-\hat{a}\hat{a}^\dagger-\hat{a}^\dagger\hat{a}\right]$ $=-\dfrac{\hbar m\omega}{2}\left[\hat{a}^2+\hat{a}^{\dagger 2}-2\hat{a}^\dagger\hat{a}-1\right]$

$\langle\hat{p}^2\rangle=-\dfrac{\hbar m\omega}{2}\times\dfrac{1}{2}[\langle 0|\hat{a}^2|0\rangle+\langle 0|\hat{a}^2|1\rangle+\langle 1|\hat{a}^2|0\rangle+\langle 1|\hat{a}^2|1\rangle+\langle 0|\hat{a}^{\dagger 2}|0\rangle+\langle 1|\hat{a}^{\dagger 2}|1\rangle+\langle 0|\hat{a}^{\dagger 2}|1\rangle+\langle 1|\hat{a}^{\dagger 2}|0\rangle$

$-2\left(\langle 0|\hat{a}^\dagger a\rangle+\langle 1|\hat{a}^\dagger\hat{a}|1\rangle+\langle 0|\hat{a}^\dagger\hat{a}|1\rangle+\langle 1|\hat{a}^\dagger a|0\rangle-\left(\langle 0|0\rangle+\langle 1|1\rangle\right)+\langle 0|1\rangle+\langle 1|0\rangle\right)$

$=-\dfrac{\hbar m\omega}{4}\left[-2(0+1)-1(1+1)\right]==\hbar m\omega$ $\Rightarrow\ \Delta p=\sqrt{\hbar m\omega}$

Correct answer is (c).

5. The wavefunction of a particle at t = 0 is given by $|\psi(0)\rangle = \frac{1}{\sqrt{2}}[|u_1\rangle + |u_2\rangle]$, where $|u_1\rangle$ and $|u_2\rangle$ are the normalized eigenstates with eigenvalues E_1 and E_2 respectively, $(E_2 > E_1)$. The shortest time after which $|\psi(t)\rangle$ will become orthogonal to $|\psi(0)\rangle$ is **[CSIR Dec 2011]**

(a) $-\frac{\hbar\pi}{(E_2 - E_1)}$ (b) $\frac{\hbar\pi}{(E_2 - E_1)}$ (c) $\frac{\sqrt{2}\hbar\pi}{(E_2 - E_1)}$ (d) $\frac{2\hbar\pi}{(E_2 - E_1)}$

Soln. $|\psi(0)\rangle = \frac{1}{\sqrt{2}}[|u_1\rangle + |u_2\rangle] \Rightarrow |\psi(t)\rangle = \frac{1}{\sqrt{2}}\left[e^{\frac{-iE_1t}{\hbar}}|u_1\rangle + e^{\frac{-iE_2t}{\hbar}}|u_2\rangle\right]$

Since, $|\psi(t)\rangle$ will become orthogonal to $|\psi(0)\rangle$ i.e. $\langle\psi(0)|\psi(t)\rangle = 0$

$$\Rightarrow \frac{1}{2}\left(e^{\frac{-iE_1t}{\hbar}} + e^{\frac{-iE_2t}{\hbar}}\right) = 0 \Rightarrow e^{\frac{-iE_1t}{\hbar}} = -e^{\frac{-iE_2t}{\hbar}} \Rightarrow e^{\frac{(E_2-E_1)t}{\hbar}} = -1 = e^{-i(2n+1)\pi}$$

$$\Rightarrow \frac{(E_2 - E_1)t}{\hbar} = (2n+1)\pi \Rightarrow t = \frac{(2n+1)\pi\hbar}{(E_2 - E_1)}$$

Therefore, the minimum time will be $t = \frac{\pi\hbar}{E_2 - E_1}$

Correct answer is (b)

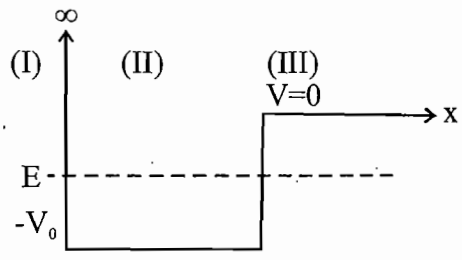
6. A particle in one-dimension is in the potential

$$V(x) = \begin{cases} \infty & \text{if } x < 0 \\ -V_0 & \text{if } 0 \le x \le \ell \\ 0 & \text{if } x > \ell \end{cases}$$

If there is at least one bound state, the minimum depth of the potential is **[CSIR June 2012]**

(a) $\frac{\hbar^2\pi^2}{8m\ell^2}$ (b) $\frac{\hbar^2\pi^2}{2m\ell^2}$ (c) $\frac{2\hbar^2\pi^2}{m\ell^2}$ (d) $\frac{\hbar^2\pi^2}{m\ell^2}$

Soln. $V(x) = \begin{cases} \infty & \text{if } x < 0 \\ -V_0 & \text{if } 0 < x < \ell \\ 0 & \text{if } x > \ell \end{cases}$



Region I: $\psi_I = 0$

Region II: $\frac{d^2\psi_{II}}{dx^2} + \frac{2m}{\hbar^2}(E + V_0)\psi_{II} = 0 \Rightarrow \frac{d^2\psi_{II}}{dx^2} + k_I^2\psi_{II} = 0,$ where $k_I^2 = \frac{2m}{\hbar^2}(E + V_0)$

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Solution: $\psi_{II} = A\sin k_1 x + B\cos k_1 x$

Region III: $\dfrac{d^2\psi_{III}}{dx^2} + \dfrac{2mE}{\hbar^2}\psi_{III} = 0 \Rightarrow \dfrac{d^2\psi_{III}}{dx^2} - k_2^2\psi_{III} = 0$, where $k_2^2 = \dfrac{-2mE}{\hbar^2}$

Solution: $\psi_{III} = Ce^{k_2 x} + De^{-k_2 x}$

Since, the wavefunction should be finite everywhere in space, therefore $C = 0$ and $\psi_{III} = De^{-k_2 x}$

Boundary conditions:

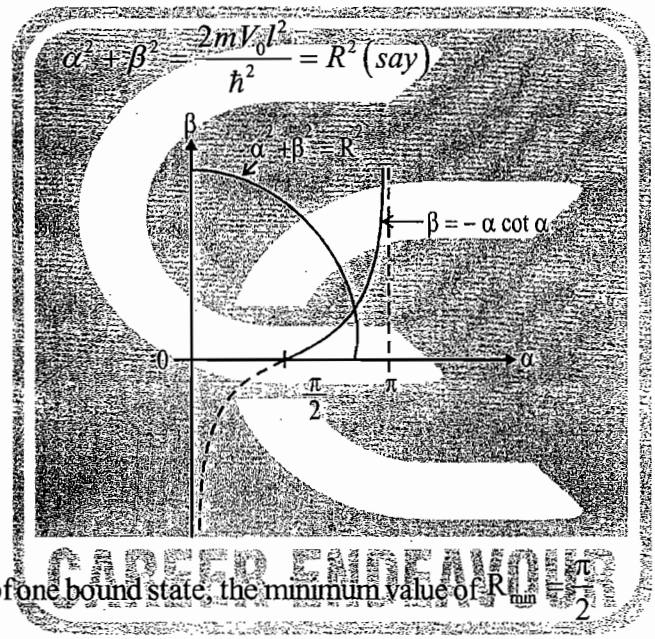
(i) $\psi_I|_{x=0} = \psi_{II}|_{x=0} = 0$. Therefore, $\psi_{II} = A\sin k_1 x$

(ii) $\psi_{II}|_{x=\ell} = \psi_{III}|_{x=\ell} \Rightarrow A\sin k_1\ell = De^{-k_2\ell}$

(iii) $\left.\dfrac{d\psi_{II}}{dx}\right|_{x=l} = \left.\dfrac{d\psi_{III}}{dx}\right|_{x=l} \Rightarrow k_1 A\cos k_1 l = -k_2 De^{-k_2 l}$

Using the equations from conditions (ii) and (iii), we get

$$-k_2 = k_1\cot(k_1 l) \Rightarrow k_2\ell = -k_1 l\cot(k_1 l) \Rightarrow \beta = -\alpha\cot\alpha$$



For the existance of one bound state, the minimum value of $R_{min} = \dfrac{\pi}{2}$

$$\Rightarrow R_{min}^2 = \frac{\pi^2}{4} \Rightarrow \frac{2m(V_0)_{min}\ell^2}{\hbar^2} = \frac{\pi^2}{4} \Rightarrow (V_0)_{min} = \frac{\hbar^2\pi^2}{8m\ell^2}$$

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Correct answer is (a)

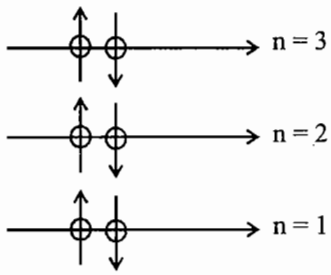
7. The minimum energy of a collection of 6 non-interacting electrons of spin $-\dfrac{1}{2}$ placed in a one dimensional infinite square well potential of width L is **[CSIR Dec 2012]**

(a) $14\pi^2\hbar^2/mL^2$ (b) $91\pi^2\hbar^2/mL^2$ (c) $7\pi^2\hbar^2/mL^2$ (d) $3\pi^2\hbar^2/mL^2$

Soln. The energy of a particle of mass 'm' in a one-dimension square well potential of width L is given by

$$E = \frac{n^2\pi^2\hbar^2}{2mL^2}, \quad n = 1, 2, 3, 4.....$$

Only two electron with spin $\dfrac{1}{2}$ can fill in the same state.



(corresponding to minimum energy)

The minimum energy of the system is

$$= 2\left(\frac{\hbar^2\pi^2}{2mL^2} + \frac{4\hbar^2\pi^2}{2mL^2} + \frac{9\hbar^2\pi^2}{2mL^2}\right) = \frac{14\pi^2\hbar^2}{mL^2}$$

Correct option is (a)

8. The energies in the ground state and first excited state of a particle of mass $m = \frac{1}{2}$ in a potential V(x) are –4 and –1, respectively, (in units in which $\hbar = 1$). If the corresponding wavefunctions are related by $\psi_1(x) = \psi_0(x)\sinh x$, then the ground state eigenfunction is **[CSIR Dec 2012]**

(a) $\psi_0(x) = \sqrt{\text{sec hx}}$ (b) $\psi_0(x) = \text{sec hx}$ (c) $\psi_0(x) = \text{sec h}^2 x$ (d) $\psi_0(x) = \text{sec h}^3 x$

Soln. The time independent schrodinger equation $\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\psi(x) = E\psi(x)$

Taking $m = \frac{1}{2}, \hbar = 1$, the equation becomes

$$\left[-\frac{d^2}{dx^2} + V(x)\right]\psi(x) = E\psi(x)$$

For ground state, $\left[-\frac{d^2}{dx^2} + V(x)\right]\psi_0(x) = -4\psi_0(x)$

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For first excited state, $\left[-\frac{d^2}{dx^2} + V(x)\right]\psi_1(x) = -\psi_1(x)$

Since, $\psi_1(x) = \psi_0(x)\sinh x$

$$\Rightarrow \quad \left[-\frac{d^2}{dx^2} + V(x)\right]\psi_0(x)\sinh x = -\psi_0(x)\sinh x$$

$$\Rightarrow \quad -\frac{d^2}{dx^2}\left(\psi_0(x)\sinh x\right) + V(x)\psi_0(x)\sinh x = -\psi_0(x)\sinh x$$

$$\Rightarrow \quad -\frac{d}{dx}\left[\psi_0(x)\cosh x + \sinh x\frac{d\psi_0}{dx}\right] + V(x)\psi_0\sinh x = -\psi_0(x)\sinh x$$

$$\Rightarrow \quad -\psi_0(x)\sinh x - \cosh x\frac{d\psi_0}{dx} - \cosh x\frac{d\psi_0}{dx} - \sinh x\frac{d^2\psi_0}{dx^2} + V(x)\psi_0(x)\sinh x = -\psi_0(x)\sinh x$$

$$\Rightarrow \quad -2\cosh x\frac{d\psi_0}{dx}-\sinh x\frac{d^2\psi_0}{dx^2}+V(x)\psi_0(x)\sinh x=0$$

$$\Rightarrow \quad \frac{d^2\psi_0}{dx^2}+\frac{2\cosh x}{\sinh x}\frac{d\psi_0}{dx}=V(x)\psi_0(x)$$

Using the Schrodinger equation for ground state, we get

$$\Rightarrow \quad \frac{d^2\psi_0}{dx^2}+\frac{2\cosh x}{\sinh x}\frac{d\psi_0}{dx}=\frac{d^2\psi_0}{dx^2}-4\psi_0(x)$$

$$\Rightarrow \quad \frac{d\psi_0}{dx}=-2\frac{\sinh x}{\cosh x}\psi_0(x) \quad \Rightarrow \frac{d\psi_0}{\psi_0}=-\frac{2\sinh x}{\cosh x}dx$$

$$\Rightarrow \quad \ln\psi_0=\ln\sec h^2x+\ln C$$

Therefore, the ground state eigenfunction will be $\psi_0(x)=C\sec h^2x$

Correct option is (c)

9. Let $|0\rangle$ and $|1\rangle$ denote the normalized eigenstates corresponding to the ground and the first excited states of a one-dimensional harmonic oscillator. The uncertainty Δx in the state $\frac{1}{\sqrt{2}}(|0\rangle+|1\rangle)$ is :

[CSIR Dec 2012]

(a) $\Delta x=\sqrt{\hbar/2m\omega}$ (b) $\Delta x=\sqrt{\hbar/m\omega}$ (c) $\Delta x=\sqrt{2\hbar/m\omega}$ (d) $\Delta x=\sqrt{\hbar/4m\omega}$

Soln. $\langle x\rangle=\langle\psi|\hat{x}|\psi\rangle=\frac{1}{2}\left[\langle 0|\hat{x}|0\rangle+\langle 1|\hat{x}|1\rangle+\langle 0|\hat{x}|1\rangle+\langle 1|\hat{x}|0\rangle\right]$

$$=\sqrt{\frac{\hbar}{2m\omega}}\times\frac{1}{2}\left[\langle 0|(\hat{a}+\hat{a}^\dagger)|0\rangle+\langle 1|(\hat{a}+\hat{a}^\dagger)|1\rangle+\langle 0|(\hat{a}+\hat{a}^\dagger)|1\rangle+\langle 1|(\hat{a}+\hat{a}^\dagger)|0\rangle\right]$$

$$=\sqrt{\frac{\hbar}{2m\omega}}\frac{1}{2}[0+0+1+1]=\sqrt{\frac{\hbar}{2m\omega}}$$

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$$\hat{x}^2=\left(\sqrt{\frac{\hbar}{2m\omega}}\right)^2\left[\hat{a}^2+\hat{a}^{\dagger 2}+\hat{a}\hat{a}^\dagger+\hat{a}^\dagger\hat{a}\right]=\frac{\hbar}{2m\omega}\left[\hat{a}^2+\hat{a}^{\dagger 2}+2\hat{a}^\dagger\hat{a}+1\right]$$

$$\langle x^2\rangle=\frac{\hbar}{2m\omega}\times\frac{1}{2}[\langle 0|\hat{a}^2|0\rangle+\langle 0|\hat{a}^2|1\rangle+\langle 1|\hat{a}^2|0\rangle+\langle 1|\hat{a}^2|1\rangle+\langle 0|\hat{a}^{\dagger 2}|0\rangle+\langle 1|\hat{a}^{\dagger 2}|1\rangle+\langle 0|\hat{a}^{\dagger 2}|1\rangle+\langle 1|\hat{a}^{\dagger 2}|0\rangle$$
$$+2\left(\langle 0|\hat{a}^\dagger a|0\rangle+\langle 1|\hat{a}^\dagger\hat{a}|1\rangle+\langle 0|\hat{a}^\dagger\hat{a}|1\rangle+\langle 1|\hat{a}^\dagger a|0\rangle\right)+\left(\langle 0|0\rangle+\langle 1|1\rangle+\langle 0|1\rangle+\langle 1|0\rangle\right)$$

$$\langle x^2\rangle=\frac{\hbar}{2m\omega}\frac{1}{2}[2+1+1]=\frac{\hbar}{m\omega}$$

Therefore, $\Delta x=\sqrt{\langle x^2\rangle-\langle x\rangle^2}=\sqrt{\frac{\hbar}{2m\omega}}$

Correct option is (a)

10. Consider the normalized state $|\psi\rangle$ of a particle in a one-dimensional harmonic oscillator: $|\psi\rangle = b_1|0\rangle + b_2|1\rangle$ where $|0\rangle$ and $|1\rangle$ denote the ground and first excited states respectively, and b_1 and b_2 are real constants. The expectation value of the displacement x in the state $|\psi\rangle$ will be a minimum when **[CSIR June 2013]**

(a) $b_2 = 0, (b_1 = 1)$ (b) $b_2 = \frac{1}{\sqrt{2}} b_1$ (c) $b_2 = \frac{1}{2} b_1$ (d) $b_2 = -b_1$

Soln. Given : Normalized state $|\psi\rangle$ of a particle in a one-dimensional harmonic oscillator is

$|\psi\rangle = b_1|0\rangle + b_2|1\rangle$

Normalization condition : $b_1^2 + b_2^2 = 1$

Here $|0\rangle \rightarrow$ ground state

$|1\rangle \rightarrow$ first excited state

Expectation value of the displacement x in the state $|\psi\rangle = \langle\psi|x|\psi\rangle$

$= b_1^2 \langle 0|x|0\rangle + b_2^2 \langle 1|x|1\rangle + b_1 b_2 \langle 0|x|1\rangle + b_2 b_1 \langle 1|x|0\rangle$

Since, x is an odd function, therefore first two terms of the aboye expression will be zero.

$P = \langle\psi|x|\psi\rangle = b_1 b_2 \langle 0|x|1\rangle + b_2 b_1 \langle 1|x|0\rangle$

$= b_1 b_2 \sqrt{\frac{\hbar}{2m\omega}} \left[\langle 0|\hat{a} + \hat{a}^\dagger|1\rangle + \langle 1|\hat{a} + \hat{a}^\dagger|0\rangle\right]$

$= \sqrt{\frac{\hbar}{2m\omega}} b_1 b_2 \left[\langle 0|\sqrt{1}|0\rangle + \langle 0|\sqrt{2}|2\rangle + 0 + \langle 1|\sqrt{1}|1\rangle\right]$

$= \sqrt{\frac{\hbar}{2m\omega}} b_1 b_2 (1+1) = 2 b_1 b_2 \sqrt{\frac{\hbar}{2m\omega}}$

Now P will be minimum if $b_1 b_2$ is minimum.

Therefore, $b_1 b_2 = \frac{1}{4}\left[(b_1 + b_2)^2 - (b_1 - b_2)^2\right]$ is minimum (say)

So, $b_1 b_2$ will be minimum if $b_2 = 0$ or $b_1 = 0$

Case 1: $b_1 = 0 \Rightarrow b_2 = 1$

Case 2: $b_2 = 0 \Rightarrow b_2 = 1$ [Due to normalization condition $b_1^2 + b_2^2 = 1$]

So, correct option should be (a)

In the answer key correct option is given to be (d) i.e. $b_1 = b_2$

If $b_1 = b_2 \Rightarrow b_1 b_2$ will be maximum and its maximum value will be b_1^2 or b_2^2 then, $\langle\psi|x|\psi\rangle$ will be maximum and its maximum value will be $2b_1^2\sqrt{\frac{\hbar}{2m\omega}}$ or $2b_2^2\sqrt{\frac{\hbar}{2m\omega}}$

Correct answer is (a)

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11. A particle is in the ground state of an infinite square well potential given by,

$$V(x)=\begin{cases}0 & \text{for } -a\le x\le a\\ \infty & \text{otherwise}\end{cases}$$

The probability to find the particle in the interval between $-\frac{a}{2}$ and $\frac{a}{2}$ is **[CSIR Dec 2013]**

(a) $\frac{1}{2}$ (b) $\frac{1}{2}+\frac{1}{\pi}$ (c) $\frac{1}{2}-\frac{1}{\pi}$ (d) $\frac{1}{\pi}$

Soln. Given : $V(x)=\begin{cases}0 & \text{for } -a\le x\le a\\ \infty & \text{otherwise}\end{cases}$

Symmetrical infinite potential well of width '2a'

Ground state wavefunction of the particle $\psi_1(x)=\sqrt{\frac{2}{2a}}\cos\left(\frac{\pi x}{2a}\right)$

Probability of finding the particle in the interval between $-\frac{a}{2}$ to $\frac{a}{2}$ is

$$P=\int_{-a/2}^{a/2}\psi'_1\psi_1 dx=\frac{1}{a}\int_{-a/2}^{a/2}\cos^2\left(\frac{\pi x}{2a}\right)dx=\frac{1}{2a}\int_{-a/2}^{a/2}\left[1+\cos\left(\frac{\pi x}{a}\right)\right]dx$$

$$=\frac{1}{2a}\left[x+\frac{a}{\pi}\sin\left(\frac{\pi x}{a}\right)\right]_{-a/2}^{a/2}=\frac{1}{2a}\left[a+\frac{2a}{\pi}\right]=\frac{1}{2}+\frac{1}{\pi}$$

Correct answer is (b)

12. A particle in the infinite square well

$$V(x)=\begin{cases}0 & 0<x<a\\ \infty & \text{otherwise}\end{cases}$$

is prepared in a state with the wavefunction

$$\psi(x)=\begin{cases}A\sin^3\left(\frac{\pi x}{a}\right) & 0<x<a\\ 0 & \text{otherwise}\end{cases}$$

The expectation value of the energy of the particle is **[CSIR June 2014]**

(a) $\frac{5\hbar^2\pi^2}{2ma^2}$ (b) $\frac{9\hbar^2\pi^2}{2ma^2}$ (c) $\frac{9\hbar^2\pi^2}{10ma^2}$ (d) $\frac{\hbar^2\pi^2}{2ma^2}$

Soln. $\psi(x)=A\sin^3\left(\frac{\pi x}{a}\right)=\frac{3A}{4}\sin\left(\frac{\pi x}{a}\right)-\frac{A}{4}\sin\left(\frac{3\pi x}{a}\right)$

$$\Rightarrow\quad \psi(x)=\frac{3A}{4}\sqrt{\frac{a}{2}}\left[\sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right)\right]-\frac{A}{4}\sqrt{\frac{a}{2}}\left[\sqrt{\frac{2}{a}}\sin\left(\frac{3\pi x}{a}\right)\right]$$

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Since, $\psi(x)$ is normalized, then

$$\left[\frac{3A}{4}\sqrt{\frac{a}{2}}\right]^2+\left[\frac{A}{4}\sqrt{\frac{a}{2}}\right]^2=1 \quad \Rightarrow \frac{9A^2}{16}\cdot\frac{a}{2}+\frac{A^2}{16}\cdot\frac{a}{2}=1 \Rightarrow \quad A=\sqrt{\frac{16}{5a}}=\frac{4}{\sqrt{5a}}$$

Therefore, $\psi(x)=\frac{3}{\sqrt{10}}\psi_1+\frac{1}{\sqrt{10}}\psi_3$

Expectation value of energy $=\langle E\rangle = P_1E_1+P_3E_3=\frac{9}{10}\frac{\pi^2\hbar^2}{2ma^2}+\frac{1}{10}\frac{9\pi^2\hbar^2}{2ma^2}=\frac{9\pi^2\hbar^2}{10ma^2}$

Correct answer is (c)

13. Let ψ_1 and ψ_2 denote, the normalized eigenstates of a particle with energy eigenvalues E_1 and E_2 respectively, with $E_2 > E_1$. At time $t=0$ the particle is prepared in a state $\Psi(t=0)=\frac{1}{\sqrt{2}}(\psi_1+\psi_2)$. The shortest time T at which $\Psi(t=T)$ will be orthogonal to $\Psi(t=0)$ is

[CSIR Dec 2014]

(a) $\frac{2\hbar\pi}{(E_2-E_1)}$ (b) $\frac{\hbar\pi}{(E_2-E_1)}$ (c) $\frac{\hbar\pi}{2(E_2-E_1)}$ (d) $\frac{\hbar\pi}{4(E_2-E_1)}$

Soln. Given: At $t=0$, the wavefunction of the particle is $\psi(t=0)=\frac{1}{\sqrt{2}}(\psi_1+\psi_2)$

The wave function of the particle at $t=T$ is $\psi(t=T)=\frac{1}{\sqrt{2}}\left(\psi_1 e^{-iE_1T/\hbar}+\psi_2 e^{-iE_2T/\hbar}\right)$

Since, $\psi(t=T)$ and $\psi(t=0)$ are orthogonal, then

$$\langle\psi(t=T)|\psi(t=0)\rangle=0$$

$$\Rightarrow \frac{1}{2}e^{iE_1T/\hbar}\langle\psi_1|\psi_1\rangle+\frac{1}{2}e^{iE_1T/\hbar}\langle\psi_1|\psi_2\rangle+\frac{1}{2}e^{iE_2T/\hbar}\langle\psi_2|\psi_1\rangle+\frac{1}{2}e^{iE_2T/\hbar}\langle\psi_2|\psi_2\rangle=0$$

$$\Rightarrow \frac{1}{2}e^{iE_1T/\hbar}+\frac{1}{2}e^{iE_2T/\hbar}=0 \Rightarrow e^{iE_1T/\hbar}+e^{iE_2T/\hbar}=0$$

$$\Rightarrow e^{iE_1T/\hbar}=-e^{iE_2T/\hbar} \qquad \Rightarrow e^{i(E_2-E_1)T/\hbar}=-1=e^{i(2n+1)\pi}$$

$$\Rightarrow \frac{(E_2-E_1)T}{\hbar}=(2n+1)\pi \quad \Rightarrow T=\frac{(2n+1)\pi\hbar}{E_2-E_1}$$

For shortest time taking $n=0$, $T=\frac{\pi\hbar}{E_2-E_1}$

Correct Option is (b)

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14. Let $|\psi\rangle = c_0|0\rangle + c_1|1\rangle$ (where c_0 and c_1 are constants with $c_0^2 + c_1^2 = 1$) be a linear combination of the wavefunctions of the ground and first excited states of the one-dimensional harmonic oscillator. For what value of c_0 is the expectation value $\langle x\rangle$ a maximum? **[CSIR Dec 2014]**

(a) $\langle x\rangle = \sqrt{\frac{\hbar}{m\omega}},\ c_0 = \frac{1}{\sqrt{2}}$ (b) $\langle x\rangle = \sqrt{\frac{\hbar}{2m\omega}},\ c_0 = \frac{1}{2}$

(c) $\langle x\rangle = \sqrt{\frac{\hbar}{2m\omega}},\ c_0 = \frac{1}{\sqrt{2}}$ (d) $\langle x\rangle = \sqrt{\frac{\hbar}{m\omega}},\ c_0 = \frac{1}{2}$

Soln. Given: $|\psi\rangle = c_0|0\rangle + c_1|1\rangle$ with $|c_0|^2 + |c_1|^2 = 1$

Expectation value of position =

$$\langle x\rangle = \langle\psi|x|\psi\rangle = \left[c_0\langle 0| + c_1\langle 1|\right]\left[\sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a} + \hat{a}^\dagger\right)\right]\left[c_0|0\rangle + c_1|1\rangle\right]$$

Using the relations, $\hat{a}|n\rangle = \sqrt{n}|n-1\rangle$ and $\hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$, we get

$$= \sqrt{\frac{\hbar}{2m\omega}}\left[c_0\langle 0| + c_1\langle 1|\right]\left[c_1|0\rangle + c_0|1\rangle + c_1\sqrt{2}|2\rangle\right]$$

$$= \sqrt{\frac{\hbar}{2m\omega}}\left[c_0c_1 + c_1c_0\right] = 2c_0c_1\sqrt{\frac{\hbar}{2m\omega}}$$

The expectation value of position $\langle x\rangle$ is maximum when c_0c_1 is maximum. The maximum value of c_0c_1 occurs for $c_0 = c_1$. Since, $c_0^2 + c_1^2 = 1$, then $c_0 = c_1 = \frac{1}{\sqrt{2}}$

Therefore, the maximum of expctation value of position is $\langle x\rangle = \sqrt{\frac{\hbar}{2m\omega}}$

Correct Option is (c)

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PRACTICE SET

1. If the wave function of a particle trapped in space between $x = 0$ and $x = L$ is given by $\psi(x) = A\sin\left(\frac{2\pi x}{L}\right)$, where A is a constant, for which value(s) of x will the probability of finding the particle be the maximum? **[GATE 2002]**

(a) $\frac{L}{4}$ (b) $\frac{L}{2}$ (c) $\frac{L}{6}$ and $\frac{L}{3}$ (d) $\frac{L}{4}$ and $\frac{3L}{4}$

2. The energy density of states of an electron in a one dimensional potential well of infinitely high walls is (the symbols have their usual meaning) **[GATE 2003]**

(a) $L\sqrt{m}/\left[\pi\hbar\sqrt{(2E)}\right]$ (b) $Lm/\left(\pi\hbar\sqrt{E}\right)$

(c) $Lm/\left[\pi\hbar\sqrt{(2E)}\right]$ (d) $L\sqrt{m}/(2\pi\hbar E)$

3. A free particle with energy E whose wave-function is a plane wave with wavelength λ enters a regionof constant potential V>0 where the wavelength of the particle is 2λ. The ratio (V/E) is: **[GATE 2003]**

(a) 1/2 (b) 2/3 (c) 3/4 (d) 4/5

Common data for Q. 4 and Q. 5

A particle is confined to the region $0 < x < L$ in one dimension. **[GATE 2004]**

4. If the particle is in the first excited state, then the probability of finding the particle is maximum at

(a) $x = \frac{L}{6}$ (b) $x = \frac{L}{2}$ (c) $x = \frac{L}{3}$ (d) $x = \frac{L}{4}$ and $\frac{3L}{4}$

5. If the particle is in the lowest energy state, then the probability of finding the particle in the region 0 to $\frac{L}{4}$ is:

(a) $\frac{1}{4} - \frac{1}{(2\pi)}$ (b) $\frac{1}{4}$ (c) $\frac{1}{4} + \frac{1}{(2\pi)}$ (d) $\frac{1}{2}$

6. A beam of monoenergetic particles having speed v is described by the wave funcion $\psi(x) = u(x)\exp(ikx)$, where $u(x)$ is a real function. This corresponds to a current density **[GATE 2004]**

(a) $u^2(x)v$ (b) v (c) zero (d) $u^2(x)$

7. A one-dimensional harmonic oscillator carrying a charge $-q$ is placed in a uniform electric field $\vec{E}$ along positive axis. The corresponding Hamiltonian operator is **[GATE 2005]**

(a) $\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}kx^2 + qEx$ (b) $\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}kx^2 - qEx$

(c) $-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}kx^2 + qEx$ (d) $-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}kx^2 - qEx$

8. A partricle is incident with a constant energy E on a one-dimensional potential barrier as shown in the figure. **[GATE 2005]**

The wavefunctions in regions I and II are respectively

(a) decaying, oscillatory

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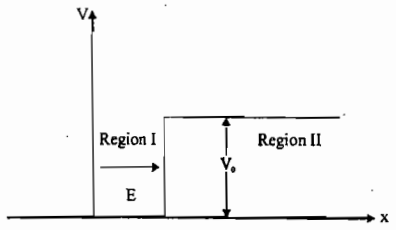
(b) oscillatory, oscillatroy

(c) oscillatory, decaying
(d) decaying, decaying.

9. A one-dimensional harmonic oscillator is in the state



$$\psi(x)=\frac{1}{\sqrt{14}}\left[3\psi_0(x)-2\psi_1(x)+\psi_2(x)\right]$$

Where $\psi_0(x),\psi_1(x)$ and $\psi_2(x)$ are the ground, first excited and second excited states, respectively. The probability of finding the oscillator in the ground state is: **[GATE 2006]**

(a) 0 (b) $\frac{3}{\sqrt{14}}$ (c) $\frac{9}{14}$ (d) 1

10. A free particle is moving in +x direction with a linear momentum p. The wavefunction of the particle normalised in a length L is: **[GATE 2006]**

(a) $\frac{1}{\sqrt{L}}\sin\frac{p}{h}x$ (b) $\frac{1}{\sqrt{L}}\cos\frac{p}{h}x$ (c) $\frac{1}{\sqrt{L}}e^{-i\frac{p}{h}x}$ (d) $\frac{1}{\sqrt{L}}e^{i\frac{p}{h}x}$

Common data for Q. 11, Q. 12 and Q. 13

A particle of mass m is confined in the ground state of a one-diemensional box, extending from $x=-2L$ to $x=+2L$. The wavefunction of the particle in this state is $\psi(x)=\psi_0\cos\frac{\pi x}{4L}$. Where ψ_0 is a constant **[GATE 2007]**

11. The normalization factor ψ_0 of this wavelength is:

(a) $\sqrt{\frac{2}{L}}$ (b) $\sqrt{\frac{1}{4L}}$ (c) $\sqrt{\frac{1}{2L}}$ (d) $\sqrt{\frac{1}{L}}$

12. The energy eigenvalue corresponding to this state is:

(a) $\frac{\hbar^2\pi^2}{2mL^2}$ (b) $\frac{\hbar^2\pi^2}{4mL^2}$ (c) $\frac{\hbar^2\pi^2}{16mL^2}$ (d) $\frac{\hbar^2\pi^2}{32mL^2}$

13. The expectation value of p^2 (p is the momentum operator) in this state is:

(a) 0 (b) $\frac{\hbar^2\pi^2}{32L^2}$ (c) $\frac{\hbar^2\pi^2}{16L^2}$ (d) $\frac{\hbar^2\pi^2}{8L^2}$

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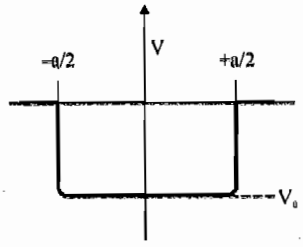
14. There are only three bound states for a particle of mass m in a one-dimensional potential well of the form shown in the figure. The depth V_0 of the potential satisfies **[GATE 2007]**



(a) $\frac{2\pi^2\hbar^2}{ma^2}<V_0<\frac{9\pi^2\hbar^2}{2ma^2}$ (b) $\frac{2\pi^2\hbar^2}{ma^2}<V_0<\frac{2\pi^2\hbar^2}{ma^2}$ (c) $\frac{2\pi^2\hbar^2}{ma^2}<V_0<\frac{8\pi^2\hbar^2}{ma^2}$ (d) $\frac{2\pi^2\hbar^2}{ma^2}<V_0<\frac{50\pi^2\hbar^2}{ma^2}$

15. For a particle of mass m in a one-dimensional harmonic oscillator potential of the form $V(x)=\frac{1}{2}m\omega^2x^2$, the first excited energy eigen state is $\psi(x)=xe^{-ax^2}$. The value of a is **[GATE 2007]**

(a) $\frac{m\omega}{4\hbar}$ (b) $\frac{m\omega}{3\hbar}$ (c) $\frac{m\omega}{2\hbar}$ (d) $\frac{2m\omega}{3\hbar}$

16. A particle with energy E is in a time-independent double well potential as shown in the figure. Which of the following statements about the particle is NOT correct? **[GATE 2007]**
(a) The particle will always be in a bound state.
(b) The probability of finding the particle in one well will be time-dependent.
(c) The particle will be confined to any one of the wells.
(d) The particle can tunnel from one well to the other, and back.

17. The energy levels of a particle of mass m in a potential of the form **[GATE 2007]**

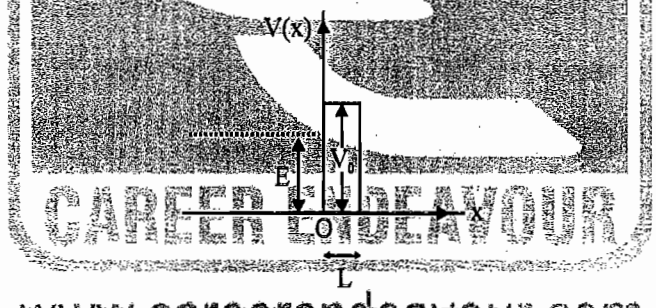
$$V(x)=\infty, \quad x\le 0$$
$$=\frac{1}{2}m\omega^2x^2, \quad x>0$$

are given, in terms of quantum number $n=0,1,2,3.....$, by

(a) $\left(n+\frac{1}{2}\right)\hbar\omega$ (b) $\left(2n+\frac{1}{2}\right)\hbar\omega$ (c) $\left(2n+\frac{3}{2}\right)\hbar\omega$ (d) $\left(n+\frac{3}{2}\right)\hbar\omega$

Common data for Q.18, Q. 19 and Q. 20

A beam of identical particles of mass m and energy E is incident from left on a potential barrier of width L (between $0<x<L$) and height V_0 as shown in the figure $(E<V_0)$ **[GATE 2008]**



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For $x>L$, there is tunneling with a transmission coefficient $T>0$. Let A_0, A_R and A_T denote the amplitudes for the incident, reflected and the transmitted waves, respectively.

18. The ratio of the reflected to the incident amplitude $\frac{A_R}{A_0}$ is:

(a) $1-\frac{A_R}{A_0}$ (b) $\sqrt{1-T}$ in magnitude

(c) A real negative number (d) $\sqrt{\left(1-\left|\frac{A_T}{A_0}\right|^2\right)\frac{E}{V_0-E}}$

19. Throughout $0<x<L$, the wave -function
(a) Can be chosen to be real (b) Is exponentially decaying.
(c) Is generally complex (d) Is zero.

20. Let the probability current associated with the incident wave be S_0. Let R be the reflection coefficient. Then
(a) The probabiltiy current vanishes in the classically forbidden region.
(b) The probability current is TS_0 for $x > L$.
(c) For, $x<0$, the probability current is $S_0(I+R)$
(d) For $x>L$, the probability current is complex.

21. A particle is placed in a one dimensional box of size L along the x-axis ($0<x<L$). Which of the following is true? **[GATE 2008]**

(a) In the ground state, the probability of finding the particle in the interval $\left(\frac{L}{4}, \frac{3L}{4}\right)$ is half.

(b) In the first excited state, the probability of finding the particle in the interval $\left(\frac{L}{4}, \frac{3L}{4}\right)$ is half. This also holds for states with $n = 4, 6, 8, ...$

(c) For an arbitory state $|\psi\rangle$, the probability of finding the particle in the left half of the well is half.

(d) In the ground state, the particle has a definite momentum.

22. A particle of mass m is confined in the potential,

$$V(x) = \begin{cases} \frac{1}{2}m\omega^2 x^2 & \text{for } x > 0, \\ \infty & \text{for } x \le 0 \end{cases}$$

Let the wavefunction of the particle be given by

$$\psi(x) = -\frac{1}{\sqrt{5}}\psi_0 + \frac{2}{\sqrt{5}}\psi_1,$$

where ψ_0 and ψ_1 are the eigenfunctions of the ground state and the first excited state respectively. The expectation value of the energy is: **[GATE 2010]**

(a) $\frac{31}{10}\hbar\omega$ (b) $\frac{25}{10}\hbar\omega$ (c) $\frac{13}{10}\hbar\omega$ (d) $\frac{11}{10}\hbar\omega$

Common data for Q.23 and Q.24

In a one-dimensional harmonic oscillator, φ_0, φ_1 and φ_2 are respectively the ground, first and the second excited states. These three states are normalized and are orthogonal to one another. ψ_1 and ψ_2 are two states defined by $\psi_1 = \varphi_0 + \alpha\varphi_1$ and $\psi_2 = \alpha\varphi_0 + \varphi_1 + \varphi_2$. Where α is a constant.

[GATE 2011]

23. The value of α for which ψ_2 is orthogonal to ψ_1 is:
(a) 2 (b) 1 (c) –1 (d) –2

24. For the value of α determined in Q.13, the expectation value of energy of oscillator in the state ψ_2 is:
(a) $\hbar\omega$ (b) $3\hbar\omega/2$ (c) $3\hbar\omega$ (d) $9\hbar\omega/2$

25. An electron with energy E is incident from left on a potential barrier, given by

$$V(x) = 0 \quad \text{for} \quad x < 0$$

$$= V_0 \text{ for } x > 0$$

as shown in the figure **[GATE 2011]**

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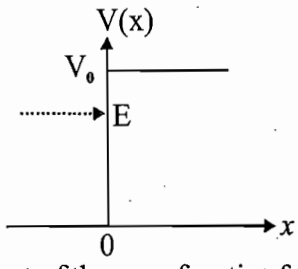
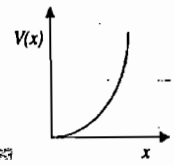


For $E < V_0$, the space part of the wavefunction for $x > 0$ is of the form

(a) $e^{\alpha x}$ (b) $e^{-\alpha x}$ (c) $e^{i\alpha x}$ (d) $e^{-i\alpha x}$

where α is a real positive quantity.

26. A particle is constrained to move in a truncated harmonic potential well ($x > 0$) as shown in the figure. Which one of the following statements is **CORRECT ?** **[GATE 2012]**



(a) The parity of the first excited state is even (b) The parity of the ground state is even

(c) The ground state energy is $\frac{1}{2}\hbar\omega$ (d) The first excited state energy is $\frac{7}{2}\hbar\omega$

27. A one dimensional harmonic oscillator is in the superposition of number state, $|n\rangle$, given by

$$|\psi\rangle = \frac{1}{2}|2\rangle + \frac{\sqrt{3}}{2}|3\rangle$$

The average energy of the oscillator in the given state is _____ $\hbar\omega$. **[GATE 2014]**

28. A particle $_1$ is confined in a one-dimensional infinite potential well with walls at $x = \pm 1$. Another Particle P_2 is confined in a one-dimensional infinite potential well with walls at $x = 0, 1$. Comparing the two particles, one can conclude that **[TIFR 2010]**

(a) the no. of nodes in the n^{th} excited state of P_1 is twice that of P_2

(b) the no. of nodes in the n^{th} excited state of P_1 is half that of P_2

(c) the energy of the n^{th} level of P_1 is the same as that of P_2

(d) the energy of the n^{th} level of P_1 is one quarter of that of P_2

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29. The wave function Ψ of a quantum mechanical system described by a Hamiltonian $\hat{H}$ can be written as a linear combination of Φ_1 and Φ_2 which are the eigenfunctions of $\hat{H}$ with eigenvalues E_1 and E_2 respectively

At $t = 0$, the system is prepared is the state $\Psi_0 = \frac{4}{5}\Phi_1 + \frac{3}{5}\Phi_2$ and then allowed to evolve with time. The wavefunction at time $T = \frac{\frac{1}{2}h}{(E_1 - E_2)}$ will be (accurate to within a phase).

[TIFR 2010]

(a) $\frac{4}{5}\Phi_1 + \frac{3}{5}\Phi_2$ (b) Φ_1 (c) $\frac{4}{5}\Phi_1 - \frac{3}{5}\Phi_2$ (d) Φ_2

(e) $\frac{3}{5}\Phi_1 + \frac{4}{5}\Phi_2$ (f) $\frac{3}{5}\Phi_1 - \frac{4}{5}\Phi_2$

30. Two identical non-interacting particles, each of mass m and spin 1/2, are placed in a one-dimensional box of length L. In quantum mechanics, the lowest possible value of the total energy of these two particles is ε_0. If, instead, four such particles are introduced into a similar one-dimensional box of length 2L, then the lowest possible value of their total energy will be **[TIFR 2011]**

(a) $2\varepsilon_0$ (b) $5\varepsilon_0/4$ (c) $3\varepsilon_0/2$ (d) ε_0

31. A particle of mass m is placed in the ground state of a one-dimensional harmonic oscillator potential of the form.

$$V(x) = \frac{1}{2}kx^2$$

where the stiffness constant k can be varied externally. The ground state wavefunction has the form $\psi(x) \propto \exp(-ax^2\sqrt{k})$ where a is a constant. If, suddenly, the parameter k is changed to 4k, the probability that the particle will remain in the ground state of the new potential is **[TIFR 2011]**

(a) 0.47 (b) 0.06 (c) 0.53 (d) 0.67

(e) 0.33 (f) 0.94

32. A particle in a one-dimensional potential has the wavefunction $\psi(x) = \frac{1}{\sqrt{a}}\exp\left(\frac{-|x|}{a}\right)$ where a is a constant. It follows that for a positive constant V_0, the potential $V(x)$ is **[TIFR 2012]**

(a) $V_0 x^2$ (b) $V_0|x|$ (c) $-V_0\delta(x)$ (d) $-V_0/|x|$

33. A harmonic oscillator has the wave function,

$$\psi(x,t) = \frac{1}{5}[3\varphi_0(x,t) - 2\sqrt{2}\varphi_1(x,t) + 2\sqrt{2}\varphi_2(x,t)]$$

where $\varphi_n(x,t)$ is the eigenfunction belonging to the n-th energy eigenvalue $\left(n+\frac{1}{2}\right)\hbar\omega$. The expectation value $\langle E \rangle$ of energy for the state $\psi(x,t)$ is **[TIFR 2013]**

(a) $1.58\hbar\omega$ (b) $0.46\hbar\omega$ (c) $\hbar\omega$ (d) $1.46\hbar\omega$

34. A particle is confined to a one-dimensional box of length L. If a vanishingly thin but strongly repulsive partition is introduced in the exact centre of the box, and the particle is allowed to come to its ground state, then the probability density for finding the particle will appear as **[TIFR 2014]**

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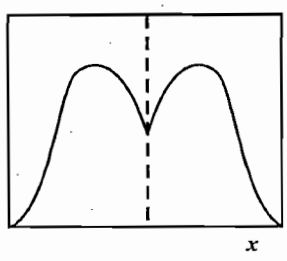
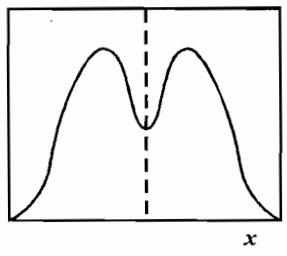
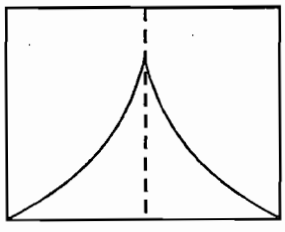
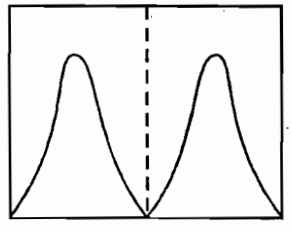
(a) 

(b) 

(c) 

(d) 

35. A particle is moving in one dimension under a potential $V(x)$ such that, for large positive values of $x, V(x) \approx kx^{\beta}$, where $k > 0$ and $\beta \geq 1$. If the wavefunction in this region has the form $\psi(x) \sim \exp(-x^{\lambda})$, which of the following is true? **[TIFR 2015]**

(a) $\lambda = \frac{\beta}{2} + 1$ (b) $\lambda = \beta$ (c) $\lambda = 2\beta - 2$ (d) $\lambda = \frac{\beta^2}{2}$

36. A one-dimensional box contains a particle whose ground state energy is ϵ. It is observed that a small disturbance causes the particle to emit a photon of energy $h\nu = 8\epsilon$, after which it is stable. Just before emission, a possible state of the particle in terms of the energy eigenstates $\{\psi_1, \psi_2, ...\}$ would be **[TIFR 2015]**

(a) $\frac{\psi_1 - \psi_2}{\sqrt{2}}$ (b) $\frac{\psi_2 + 2\psi_3}{\sqrt{5}}$ (c) $\frac{-4\psi_4 + 5\psi_5}{\sqrt{41}}$ (d) $\frac{\sqrt{2}\psi_1 - 3\psi_2 + 5\psi_5}{6}$

37. 1000 neutral spinless particles are confined in a one-dimensional box of length 100 nm. At a given instant of time, if 100 of these particle have energy $4\epsilon_0$ and the remaining 900 have energy $225\epsilon_0$, then the number of particles in the left half of the box will be approximately **[TIFR 2015]**

(a) 625 (b) 500 (c) 441 (d) 100

38. A one-dimensional quantum harmonic oscillator is in its ground state **[TIFR 2015]**

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-m\omega x^2/2\hbar}$$

Two experiments, [A] and [B], are performed on the system. In [A], the frequency ω of the oscillator is suddenly doubled, while in [B] the frequency ω is suddenly halved. If p_A and p_B denote the probability in each case that the system is found in its new ground state immediately after the frequency change, which of the following is true?

(a) $p_A = \sqrt{2}p_B$ (b) $p_A = 2p_B$ (c) $2p_A = p_B$ (d)

39. The ground state (apart from normalization) of a particle of unit mass moving in a one-dimensional potential $V(x)$ is $\exp(-x^2/2)\cosh(\sqrt{2}x)$. The potential $V(x)$, in suitable units so that $\hbar = 1$, is (up to an additive constant). **[JEST 2012]**

(a) $\frac{x^2}{2}$ (b) $\frac{x^2}{2} - \sqrt{2}x\tanh(\sqrt{2}x)$

(c) $\frac{x^2}{2} - \sqrt{2}x\tan(\sqrt{2}x)$ (d) $\frac{x^2}{2} - \sqrt{2}x\coth(\sqrt{2}x)$

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40. The grond state energy of 5 identical spin-1/2 particles which are subject to a one-dimensional simple harmonic oscillator potential of frequency ω is **[JEST 2012]**

(a) $\frac{(15/2)}{\hbar\omega}$ (b) $\frac{(13/2)}{\hbar\omega}$ (c) $\frac{(1/2)}{\hbar\omega}$ (d) $5\hbar\omega$

41. A quantum mechanical particle in a harminic oscillato potential has the initial wavefunction $\psi_0(x)+\psi_1(x)$, where ψ_0 and ψ_1 are the real wavefunctions in the ground and first excited states of the harmonic oscillator Hamiltonian. For convenience we take $m=\hbar=\omega=1$ for the oscillator. What is the probability density of finding the particle at x at time t= π? **[JEST 2013]**

(a) $\left(\psi_1(x)-\psi_0(x)\right)^2$ (b) $\left(\psi_1(x)\right)^2-\left(\psi_0(x)\right)^2$

(c) $\left(\psi_1(x)+\psi_0(x)\right)^2$ (d) $\left(\psi_1(x)\right)^2+\psi_0(x)\right)^2$

42. The lowest quantum mechanical energy of a particle confined in a one-dimensional box of size L is 2 eV. The energy of the quantum mechanical ground state for a system of three non-interacting spin-1/2 particles is **[JEST 2014]**

(a) 6 eV (b) 10 eV (c) 12 eV (d) 16 eV

43. Consider a square well of depth $-V_0$ and width a with V_0a fixed. Let $V_0 \to \infty$ and $a \to 0$. This potential well has **[JEST 2014]**

(a) No bound states (b) 1 bound state (c) 2 bound states (d) Infinitely many bound states

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Chapter 4

Angular Momentum and Spin

4.1. Orbital angular momentum :

In classical mechanics, the angular momentum $\vec{L}$ of a particle is defined as

$$\vec{L} = \vec{r} \times \vec{p} = \left(yp_z - zp_y\right)\hat{i} + \left(zp_x - xp_z\right)\hat{j} + \left(xp_y - yp_x\right)\hat{k}$$

Replacing the position and momentum co-ordinates by the equivalent quantum mechanical operators, we can have

	Cartesian co-ordinates	Spherical Polar Co-ordiantes
$\hat{L}_x$	$-i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)$	$i\hbar\left(\sin\phi\frac{\partial}{\partial\theta} + \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right)$
$\hat{L}_y$	$-i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)$	$i\hbar\left(-\cos\phi\frac{\partial}{\partial\theta} + \cot\theta\sin\phi\frac{\partial}{\partial\phi}\right)$
$\hat{L}_z$	$-i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$	$-i\hbar\frac{\partial}{\partial\phi}$
$\hat{L}^2$		$-\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]$

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Commmutation Relations

$$\left[\hat{L}_x, \hat{L}_y\right] = i\hbar\hat{L}_z \qquad \left[\hat{L}_y, \hat{L}_z\right] = i\hbar\hat{L}_x \qquad \left[\hat{L}_z, \hat{L}_x\right] = i\hbar\hat{L}_y$$

$$\left[\hat{L}_y, \hat{L}_x\right] = -i\hbar\hat{L}_z \qquad \left[\hat{L}_z, \hat{L}_y\right] = -i\hbar\hat{L}_x \qquad \left[\hat{L}_x, \hat{L}_z\right] = -i\hbar\hat{L}_y$$

i.e. the components of the orbital angular momentums cannot be measured simultaneously accurately.

$$\left[\hat{L}^2, \hat{L}_x\right] = 0 \qquad \left[\hat{L}^2, \hat{L}_y\right] = 0 \qquad \left[\hat{L}^2, \hat{L}_z\right] = 0$$

i.e. square of the orbital angular momentum commutes with any one of components of the orbital angular momentum.

$$\left[\hat{L}_x, \hat{p}_x\right] = 0 \qquad \left[\hat{L}_y, \hat{p}_y\right] = 0 \qquad \left[\hat{L}_y, \hat{p}_z\right] = 0$$

$$\left[\hat{L}_x, \hat{p}_y\right] = i\hbar\hat{p}_z \qquad \left[\hat{L}_y, \hat{p}_z\right] = i\hbar\hat{p}_x \qquad \left[\hat{L}_z, \hat{p}_x\right] = i\hbar\hat{p}_y$$

$$\left[\hat{L}_x, \hat{x}\right] = 0 \qquad \left[\hat{L}_y, \hat{y}\right] = 0 \qquad \left[\hat{L}_z, \hat{z}\right] = 0$$

$$\left[\hat{L}_x, \hat{y}\right] = i\hbar\hat{z} \qquad \left[\hat{L}_y, \hat{z}\right] = i\hbar\hat{x} \qquad \left[\hat{L}_z, \hat{x}\right] = i\hbar\hat{y}$$

Eigevalues and eigenfunctions of $\hat{L}^2$ and $\hat{L}_z$:

Since, the commutator bracket $\left[\hat{L}^2, \hat{L}_z\right] = 0$, therefore $\hat{L}^2$ and $\hat{L}_z$ can be measured simultaneously accurately and both have simultaneous eigenfunctions or eigenkets. Denoting the simultaneous eigenkets by $|l, m_l\rangle$ (where l and m_l are the orbital quantum number and orbital magnetic quantum number respectively), the eigenvalue equation for $\hat{L}^2$ and $\hat{L}_z$ can be written as

$$\hat{L}^2|l, m_l\rangle = l(l+1)\hbar^2|l, m_l\rangle$$

$$\hat{L}_z|l, m_l\rangle = m_l\hbar^2|l, m_l\rangle$$

Alternate form: Since, $\hat{L}^2$ and $\hat{L}_z$ depends on θ, ϕ then their eigen function is function of θ, ϕ i.e.

$$\hat{L}^2 Y_{\ell,m_l}(\theta,\phi) = \ell(\ell+1)\hbar^2 Y_{\ell,m_l}(\theta,\phi)$$

$$\hat{L}_z Y_{\ell,m_l}(\theta,\phi) = m_l\hbar Y_{\ell,m_l}(\theta,\phi)$$

where $Y_{\ell,m}(\theta,\phi)$ is said to be Spherical Harmonics and defined as

$$Y_{l,m_l}(\theta,\phi) = \varepsilon\sqrt{\left(\frac{2\ell+1}{4\pi}\right)\frac{(\ell-|m_l|)!}{(\ell+|m_l|)!}}\,P_\ell^{|m_l|}(\cos\theta)\,e^{im_l\phi}$$

where $\varepsilon = (-1)^{m_l}$ for $m_l \geq 0$ and $\varepsilon = 1$ for $m_l \leq 0$.

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Raising and Lowering Operators:

Raising Operator: $\hat{L}_+ = \hat{L}_x + i\hat{L}_y$

Lowering Operator: $\hat{L}_- = \hat{L}_x - i\hat{L}_y$

Important relations:

$$\left[\hat{L}_z, \hat{L}_+\right] = \hbar\hat{L}_+ \qquad \left[\hat{L}_z, \hat{L}_-\right] = -\hbar\hat{L}_- \qquad \left[\hat{L}_x, \hat{L}_+\right] = -\hbar\hat{L}_z \qquad \left[\hat{L}_x, \hat{L}_-\right] = \hbar\hat{L}_z$$

$$\left[\hat{L}_y, \hat{L}_+\right] = -i\hbar\hat{L}_z \qquad \left[\hat{L}_y, \hat{L}_-\right] = i\hbar\hat{L}_z \qquad \left[\hat{L}_+, \hat{L}_-\right] = 2\hbar\hat{L}_z$$

$$\hat{L}_+\hat{L}_- = \hat{L}^2 - \hat{L}_z^2 + \hbar\hat{L}_z \qquad \hat{L}_-\hat{L}_+ = \hat{L}^2 - \hat{L}_z^2 - \hbar\hat{L}_z$$

Action of $\hat{L}_+$ and $\hat{L}_-$:

$$\hat{L}_+|l, m_l\rangle = \sqrt{(\ell - m_l)(l + m_l + 1)}\hbar\,|l, m_l + 1\rangle$$

i.e. $$\hat{L}_- Y_{\ell,m_l}(\theta,\phi) = \sqrt{(\ell + m_l)(l - m_l + 1)}\;\hbar Y_{\ell,m_l-1}(\theta,\phi)$$

$$\hat{L}_-\left|l,m_l\right\rangle=\sqrt{(\ell+m_l)(l-m_l+1)}\hbar\left|l,m_l-1\right\rangle$$

i.e. $$\hat{L}_-Y_{\ell,m_l}(\theta,\phi)=\sqrt{(\ell+m_l)(l-m_l+1)}\,\hbar Y_{\ell,m_l-1}(\theta,\phi)$$

Matrix Representation of the operators:

Elements of $\hat{L}^2=\left\langle \ell',m_l'\left|\hat{L}^2\right|\ell,m_l\right\rangle=\ell(\ell+1)\hbar^2\,\delta_{\ell\ell'}\,\delta_{m_lm_l'}$, will be non-zero for $l=l'$ and $m_l=m_l'$ i.e.

$$\hat{L}^2=\begin{bmatrix}2\hbar^2&0&0\\0&2\hbar^2&0\\0&0&2\hbar^2\end{bmatrix}=2\hbar^2\begin{bmatrix}1&0&0\\0&1&0\\0&0&1\end{bmatrix}\text{ (for } l=1)$$

Elements of $\hat{L}_z=\left\langle \ell',m_l'\left|\hat{L}_z\right|\ell,m_l\right\rangle=m_l\hbar\,\delta_{\ell\ell'}\,\delta_{m_lm_l'}$, will be non-zero for $l=l'$ and $m_l=m_l'$ i.e.

$$\hat{L}_z=\begin{bmatrix}\hbar&0&0\\0&0&0\\0&0&-\hbar\end{bmatrix}=\hbar\begin{bmatrix}1&0&0\\0&0&0\\0&0&-1\end{bmatrix}\text{ (for } l=1)$$

Elements of $\hat{L}_+=\left\langle \ell',m_l'\left|\hat{L}_+\right|\ell,m_l\right\rangle=\hbar\sqrt{(\ell-m_l)(\ell+m_l+1)}\,\delta_{\ell\ell'}\,\delta_{m_l',m_l+1}$, will be non-zero for $l=l'$ and $m_l=m_l'+1$ i.e.

$$\hat{L}_+=\begin{bmatrix}0&\sqrt{2}\hbar&0\\0&0&\sqrt{2}\hbar\\0&0&0\end{bmatrix}=\sqrt{2}\hbar\begin{bmatrix}0&1&0\\0&0&1\\0&0&0\end{bmatrix}\text{ (for } l=1)$$

Elements of $\hat{L}_+=\left\langle \ell',m_l'\left|\hat{L}_-\right|\ell,m_l\right\rangle=\hbar\sqrt{(\ell+m_l)(\ell-m_l+1)}\,\delta_{\ell\ell'}\,\delta_{m_l',m_l-1}$, will be non-zero for $l=l'$ and $m_l=m_l'-1$ i.e.

$$\hat{L}_-=\sqrt{2}\hbar\begin{bmatrix}0&0&0\\1&0&0\\0&1&0\end{bmatrix}\text{ (for } l=1)$$

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Expectation values:

$$\left\langle\hat{L}_x\right\rangle=0,\ \left\langle\hat{L}_y\right\rangle=0,\ \left\langle\hat{L}_z\right\rangle=m_l\hbar$$

$$\left\langle\hat{L}_x^2\right\rangle=\left\langle\hat{L}_y^2\right\rangle=\frac{\hbar^2}{2}\left[\ell(\ell+1)-m_l^2\right],\ \left\langle\hat{L}_z^2\right\rangle=m_l^2\hbar^2$$

Example 1: Which of the following are eigenfunctions of L_z? For the cases where the function is an eigenfuntion of L_z, find the correspondence eigenvalue.

(a) $\sin\theta\, e^{i\phi}$ (b) $e^{i(\theta+\phi)}$ (c) $e^{i\theta}\sin\phi$ (d) $r^n\cos\theta$

Soln. We know, $L_z = -i\hbar\dfrac{\partial}{\partial\phi}$

(a) $-i\hbar\dfrac{\partial}{\partial\phi}\left(\sin\theta\, e^{i\phi}\right) = (-i\hbar)\sin\theta\,(i)e^{i\phi} = \hbar\sin\theta\, e^{i\phi}$

So, $\sin\theta\, e^{i\phi}$ is an eigenfunction of L_z and the corresponding eigenvalue is $\hbar$.

(b) $-i\hbar\dfrac{\partial}{\partial\phi}e^{i(\theta+\phi)} = (-i\hbar)(i)e^{i(\theta+\phi)} = \hbar e^{i(\theta+\phi)}$

So, $e^{i(\theta+\phi)}$ is an eigenfunction of L_z and the corresponding eigenvalue is $\hbar$.

(c) $-i\hbar\dfrac{\partial}{\partial\phi}\left(e^{i\theta}\sin\phi\right) = -i\hbar\, e^{i\theta}\cos\phi$

So, $e^{i\theta}\sin\theta$ is not eigenfunction of L_z.

(d) $-i\hbar\dfrac{\partial}{\partial\phi}\left(r^n\cos\theta\right) = 0 = 0.\left(r^n\cos\theta\right)$

So, $r^n\cos\theta$ is an eigenfunction of L_z and the corresponding eigenvalue is zero.

Example 2. (a) Is $\cos\theta + \sin\theta\, e^{i\phi}$ an eigenfunction of L^2 and L_z? If yes, what are the corresponding eigenvalues?

Soln. (a) We know that, $Y_{1,0}(\theta,\phi) = \sqrt{\dfrac{3}{4\pi}}\cos\theta$ and $Y_{1,1}(\theta,\phi) = \sqrt{\dfrac{3}{8\pi}}\sin\theta\, e^{i\phi}$

Thus $\cos\theta + \sin\theta\, e^{i\phi} = c_1Y_{1,0}(\theta,\phi) + c_2Y_{1,1}(\theta,\phi)$ where c_1, c_2 are constant.

$L^2\left(\cos\theta + \sin\theta\, e^{i\phi}\right) = c_1L^2Y_{1,0}(\theta,\phi) + c_2L^2Y_{1,1}(\theta,\phi)$

$= c_1 2\hbar^2Y_{1,0}(\theta,\phi) + c_2 2\hbar^2Y_{1,1}(\theta,\phi)$

$= 2\hbar^2\left[c_1Y_{1,0}(\theta,\phi) + c_2Y_{1,1}(\theta,\phi)\right] = 2\hbar^2\left[\cos\theta + \sin\theta\, e^{i\phi}\right]$

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Thus, $\cos\theta + \sin\theta\, e^{i\phi}$ is an eigenfunction of L^2 and the corresponding eigenvalue is $2\hbar^2$.

(b) $L_z\left(\cos\theta + \sin\theta\, e^{i\phi}\right) = c_1L_zY_{1,0}(\theta,\phi) + c_2L_zY_1^1(\theta,\phi) = c_1.0 + c_2\hbar Y_{1,1}(\theta,\phi) = \hbar\sin\theta\, e^{i\phi}$

Thus, $\cos\theta + \sin\theta\, e^{i\phi}$ is not an eigenfunction of L_z.

Example 3. It is given that $Y_{2,0}(\theta,\varphi) = \sqrt{\dfrac{5}{16\pi}}\left(3\cos^2\theta - 1\right)$. Find the expressions for $Y_{2,1}(\theta,\phi)$.

Soln. Expressions for L_x and L_y are given in terms of θ, ϕ. Using these,

$$L_+ = L_x + iL_y = \hbar\, e^{i\varphi}\left(\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right)$$

You can write $Y_{2,0}(\theta,\phi)$ as $|2,0\rangle$. Also, $L_+|\ell\, m\rangle = \hbar\sqrt{(\ell-m)(\ell+m+1)}\,|\ell\, m+1\rangle$

Thus, $L_+|2,0\rangle = \hbar\sqrt{6}\,|2,1\rangle \quad \Rightarrow |2,1\rangle = \frac{1}{\hbar\sqrt{6}} L_+|2,0\rangle$

$$\Rightarrow Y_{2,1}(\theta,\phi) = \frac{1}{\hbar\sqrt{6}}\hbar e^{i\phi}\left(\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right)Y_{2,0}(\theta,\phi)$$

$$= \frac{1}{\sqrt{6}}\sqrt{\frac{5}{16\pi}}e^{i\phi}\left[\frac{\partial}{\partial\theta}\left(3\cos^2\theta - 1\right) + i\cot\theta\frac{\partial}{\partial\phi}\left(3\cos^2\theta - 1\right)\right] = -\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta\, e^{i\phi}$$

Example 4. The operator associated with the measurement of the product $\ell_x\ell_y$ is $\left(L_xL_y + L_yL_x\right)/2$. Calculate the mean value of $\ell_x\ell_y$ in the state $|\ell\, m\rangle$.

Soln. We have $L_+ = L_x + iL_y$ and $L_- = L_x - iL_y$

So, $L_x = \frac{L_+ + L_-}{2}$, $L_y = \frac{L_+ - L_-}{2i}$

Thus, $L_xL_y = \frac{(L_+ + L_-)(L_+ - L_-)}{4i} = \frac{L_+^2 - L_+L_- + L_-L_+ - L_-^2}{4i}$

and $L_yL_x = \frac{(L_+ - L_-)(L_+ + L_-)}{4i} = \frac{L_+^2 + L_+L_- - L_-L_+ - L_-^2}{4i}$

So, $L_xL_y + L_yL_x = \frac{L_+^2 - L_-^2}{2i}$

The mean value of $\ell_x\ell_y$ is

$$\left\langle lm\left|\frac{L_xL_y + L_yL_x}{2}\right|\ell\, m\right\rangle = \frac{1}{4i}\left[\langle \ell\, m|L_+^2|\ell\, m\rangle - \langle \ell\, m|L_-^2|\ell\, m\rangle\right]$$

$$= \frac{1}{4i}\left[c_+^2\langle l, m_l|l, m_l+2\rangle + c_-^2\langle l, m_l|l, m_l-2\rangle\right] = 0$$

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Example 5. 3. The expectation value of the operator $\hat{L}_+$ in the state $|\psi\rangle = \frac{1}{\sqrt{3}}\left[|1,1\rangle + |1,0\rangle + |1,-1\rangle\right]$ is

(a) $\frac{2\sqrt{2}}{3}\hbar$ (b) $\frac{\sqrt{2}}{3}\hbar$ (c) $\frac{4\sqrt{2}}{3}\hbar$ (d) 0

Soln. $\langle L_+\rangle = \frac{1}{3}\left[\langle 11|L_+|11\rangle + \langle 11|L_+|10\rangle + \langle 11|L_+|1-1\rangle + \langle 10|L_+|11\rangle + \langle 10|L_+|10\rangle + \langle 10|L_+|1-1\rangle\right.$

$\left. + \langle 1-1|L_+|11\rangle + \langle 1-1|L_+|10\rangle + \langle 1-1|L_+|1-1\rangle\right]$

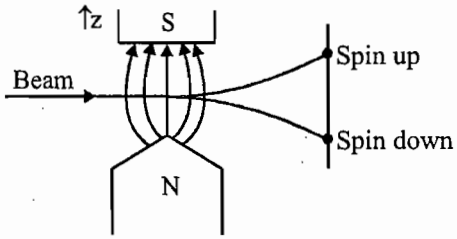
L_+ will raise the value of m to m + 1. Only those terms will survive in which this raised valued of min the ket is equal to the value of 'm' in the bra. Thus,

$$\langle L_+\rangle = \frac{1}{3}\left[\langle 11|L_+|10\rangle + \langle 10|L_+|1-1\rangle\right] = \frac{1}{3}\left[\left\langle 11\left|\sqrt{2}\hbar\right|11\right\rangle + \left\langle 10\left|\sqrt{2}\hbar\right|10\right\rangle\right] = \frac{2\sqrt{2}\hbar}{3}$$

4.2. Spin angular momentum :

Stern Gerlach Experiment

The existance of spin is first confirmed experimentally by stern and Gerlack in 1922. Using silver (Ag) atoms. Silver has 47 electrons, out of which 46 electrons form a spherically symmetric charge distribution and 47th electron occupies a '5s' orbital ($l = 0$). If the silver atom is its ground state, then its total orbital angular momentum will be zero.



Non-uniform magnetic field

If a beam of silver atoms passes through an in homogeneous (non-uniform) magnetic field (along z-direction), we would expect the following results:

(i) Classically, there will be a continuous band on the screen and the band will be symmetric about the undeflected direction $z = 0$.

(ii) Accordinh to Schrodinger's wave theory, if the atom has an orbital angular momentum 'l' then the beam will split into discrete $(2l + 1)$ components. Since, the silver atom is in ground state ($l = 0$), there will be only spot on the screen.

But, in experiments the beam splits into two distinct components.

To solve this problem, Goudsmith and Unlenbeck postulated that in addition to its orbital angular momentum, the electron possesses an intrinsic angular momentum. This angular momentum has no connection with the spaial degrees of freedom but it can be related with the internal rotational or spinning motion of the electron about its own axis. This is known as spin angular momentum which is connected with an intrinsic degree of freedom i.e. spin. Spin is a purely quantum mechanical concept with classical analog. Unlike orbital angular momentum, the spin cannot be described by a differential operator.

Consider a particle of mass 'm' and charge 'q' is moving in a circle of radius 'r'. The magnetic dipole moment due to the orbital motion of the particle will be

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$$\vec{\mu} = \frac{q}{2m}\vec{L}$$

where $\vec{L}$ is the orbital angular momentum of the particle and z-components of magnetic moment will be

$$\mu_z = \frac{q}{2m} L_z$$

For an electron the relation will be $\mu_z = -\frac{e}{2m_e} L_z$

If the electron is the eigenstates of $\hat{L}_z$, then

$$(\mu_L)_z = -\left(\frac{e}{2m_e}\right) m_l \hbar = -\mu_B m_l$$

where $\left(\frac{e\hbar}{2m_e}\right) = \mu_B$ = Bohr magneton and m_l is the orbital magnetic quantum number.

For a particular value of l, we will get $(2\ell+1)$ values of 'm_l' i.e $m_l = -l, -l+1, \ldots\ldots, 0, \ldots\ldots, l-1, l$

Similarly, if we take electron as spinning charged sphere, then the magnetic dipole moment due to the spin motion of the particle will be

$$\vec{\mu}_S = -g_s \frac{e}{2m}\vec{S}$$

where $\vec{S}$ is the spin angular momentum of the electron and g_S is the spin g-factor.
Therefore, z-components of magnetic dipole moment will be

$$(\mu_S)_z = -g_S \frac{e}{2m} S_z$$

If the electron is in an eigenstate of S_z, then

$$(\mu_S)_z = -g_s \mu_B m_s$$

where $\left(\frac{e\hbar}{2m_e}\right) = \mu_B$ = Bohr magneton and m_s is the spin magnetic quantum number.

For a particular value of s, we will get $(2s+1)$ values of 'm_s' i.e. $m_s = -s, -s+1, \ldots\ldots, 0, \ldots\ldots s-1, s$
Every fundamental particle has a specific spin $(s = 0, 1, 2, \ldots\ldots\ldots\ldots)$
Fermions: Particle having half-integer spins. Examples: quarks, electrons, protons, neutrons etc.
Bosons: Particles having integer spins. Example: Photons, pions, gravitons etc.

Therefore, there are two kinds of angular momentum of the particle i.e.

(i) Orbital angular momentum $(\vec{L})$ due to particle's orbital motion and it is characterized by two quantum numbers i.e. ℓ and its projection of z-axis 'm_ℓ' which can take values from $-\ell$ to $+\ell$.

(ii) Spin angular momentum $(\vec{S})$ due to some intrinsic motion of the particle and it is characterised by two quantum numbers i.e. s and its projection on z-axis m_s which can take values from -s to +s.
Thus, the total angular momentum can be written as

$$\vec{J} = \vec{L} + \vec{S}$$

and it is characterised by two quantum numbers i.e. j and its projection on z-axis i.e. 'm_j' which can take values from -j to +j.

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In the Stern-Gerlach experiment, the silver atom has orbital angular momentum to be zero i.e l =0 but the spin angular momentum to be 1/2 i.e. s =1/2. Therefore, total angular momentum will be

$$j = |l - s| \text{ to } |l + s| = -\frac{1}{2}, \frac{1}{2}$$

For thiis, we are getting two spots on the screen.

Pauli's Theory of Spin :

• Spin angular momentum has components S_x, S_y and S_z and the corresponding operators satisfy the foll owing commutation relation:

$$\left[\hat{S}_x, \hat{S}_y\right] = i\hbar\hat{S}_z \qquad \left[\hat{S}_y, \hat{S}_z\right] = i\hbar\hat{S}_z \qquad \left[\hat{S}_z, \hat{S}_x\right] = i\hbar\hat{S}_y$$

- $\left[\hat{S}^2, \hat{S}_z\right] = 0$ i.e. they have simultaneous eigenstate as following:

$$\hat{S}^2 |s, m_s\rangle = s(s+1)\hbar^2 |s, m_s\rangle$$

$$\hat{S}_z |s, m_s\rangle = m_s \hbar |s, m_s\rangle$$

- Raising and lowering operators are defined as following:

$$\hat{S}_\pm = \hat{S}_x \pm i\hat{S}_y$$

$$\hat{S}_+ |s, m_s\rangle = \hbar\sqrt{(s-m_s)(s+m_s+1)}\,|s, m_s+1\rangle$$

$$\hat{S}_- |s, m_s\rangle = \hbar\sqrt{(s+m_s)(s-m_s+1)}\,|s, m_s-1\rangle$$

- For a spin $\frac{1}{2}$ particles like electrons, m_s can take values $\frac{1}{2}$ and $-\frac{1}{2}$, so the possible spin states are

Spin-up state: $\chi_{1/2} = |\uparrow\rangle = \left|\frac{1}{2}, \frac{1}{2}\right\rangle$

Spin-down state: $\chi_{-1/2} = |\downarrow\rangle = \left|\frac{1}{2}, -\frac{1}{2}\right\rangle$

such that

$$\hat{S}^2 \chi_{1/2} = \frac{3}{4}\hbar^2 \chi_{1/2}, \quad \hat{S}^2 \chi_{-1/2} = \frac{3}{4}\hbar^2 \chi_{-1/2}$$

$$\hat{S}_z \chi_{1/2} = \frac{\hbar}{2}\chi_{1/2}, \quad \hat{S}_z \chi_{-1/2} = \frac{\hbar}{2}\chi_{-1/2}$$

$$\hat{S}_+ \chi_{1/2} = 0, \quad \hat{S}_+ \chi_{-1/2} = \hbar\chi_{1/2}$$

$$\hat{S}_- \chi_{1/2} = \hbar\chi_{1/2}, \quad \hat{S}_- \chi_{-1/2} = 0$$

Matrix representation of the various spin operators:

$$\hat{S}^2 = \begin{bmatrix} \left\langle \frac{1}{2}, \frac{1}{2} \middle| \hat{S}^2 \middle| \frac{1}{2}, \frac{1}{2} \right\rangle & \left\langle \frac{1}{2}, \frac{1}{2} \middle| \hat{S}^2 \middle| \frac{1}{2}, -\frac{1}{2} \right\rangle \\ \left\langle \frac{1}{2}, -\frac{1}{2} \middle| \hat{S}^2 \middle| \frac{1}{2}, \frac{1}{2} \right\rangle & \left\langle \frac{1}{2}, -\frac{1}{2} \middle| \hat{S}^2 \middle| \frac{1}{2}, -\frac{1}{2} \right\rangle \end{bmatrix} = \frac{3}{4}\hbar^2 \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$\hat{S}_z = \begin{bmatrix} \left\langle \frac{1}{2}, \frac{1}{2} \middle| \hat{S}_z \middle| \frac{1}{2}, \frac{1}{2} \right\rangle & \left\langle \frac{1}{2}, \frac{1}{2} \middle| \hat{S}_z \middle| \frac{1}{2}, -\frac{1}{2} \right\rangle \\ \left\langle \frac{1}{2}, -\frac{1}{2} \middle| \hat{S}_z \middle| \frac{1}{2}, \frac{1}{2} \right\rangle & \left\langle \frac{1}{2}, -\frac{1}{2} \middle| \hat{S}_z \middle| \frac{1}{2}, -\frac{1}{2} \right\rangle \end{bmatrix} = \frac{\hbar}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$\hat{S}_+ = \begin{bmatrix} \left\langle \frac{1}{2}, \frac{1}{2} \middle| \hat{S}_+ \middle| \frac{1}{2}, \frac{1}{2} \right\rangle & \left\langle \frac{1}{2}, \frac{1}{2} \middle| \hat{S}_+ \middle| \frac{1}{2}, -\frac{1}{2} \right\rangle \\ \left\langle \frac{1}{2}, -\frac{1}{2} \middle| \hat{S}_+ \middle| \frac{1}{2}, \frac{1}{2} \right\rangle & \left\langle \frac{1}{2}, -\frac{1}{2} \middle| \hat{S}_+ \middle| \frac{1}{2}, -\frac{1}{2} \right\rangle \end{bmatrix} = \begin{bmatrix} 0 & \hbar \\ 0 & 0 \end{bmatrix} = \hbar\begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$$

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$$\hat{S}_- = \begin{bmatrix} \left\langle \frac{1}{2},\frac{1}{2}\middle|\hat{S}_-\middle|\frac{1}{2},\frac{1}{2}\right\rangle & \left\langle \frac{1}{2},\frac{1}{2}\middle|\hat{S}_-\middle|\frac{1}{2},-\frac{1}{2}\right\rangle \\ \left\langle \frac{1}{2},-\frac{1}{2}\middle|\hat{S}_-\middle|\frac{1}{2},\frac{1}{2}\right\rangle & \left\langle \frac{1}{2},-\frac{1}{2}\middle|\hat{S}_-\middle|\frac{1}{2},-\frac{1}{2}\right\rangle \end{bmatrix} = \hbar\begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}$$

$$\hat{S}_x = \frac{1}{2}\left[\hat{S}_+ + \hat{S}_-\right] = \frac{\hbar}{2}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

$$\hat{S}_y = \frac{1}{2i}\left[\hat{S}_+ - \hat{S}_-\right] = \frac{\hbar}{2}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

Eigenvalues and eigenvectors of $\hat{S}_z$:

Eigenvalues: $\lambda = \pm\frac{\hbar}{2}$

Eigenvectors: $\chi_{1/2} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ for $\lambda = \frac{\hbar}{2}$ and $\chi_{-1/2} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$ for $\lambda = -\frac{\hbar}{2}$

Eigenvalues and eigenvectors of $\hat{S}_x$:

Eigenvalues: $\lambda = \pm\frac{\hbar}{2}$

Eigenvectors: $\frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 1 \end{bmatrix} = \frac{1}{\sqrt{2}}\left[\chi_{1/2} + \chi_{-1/2}\right]$ for $\lambda = \frac{\hbar}{2}$

and $\frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -1 \end{bmatrix} = \frac{1}{\sqrt{2}}\left[\chi_{1/2} - \chi_{-1/2}\right]$ for $\lambda = -\frac{\hbar}{2}$

Eigenvalues and eigenvectors of $\hat{S}_y$:

Eigenvalues: $\lambda = \pm\frac{\hbar}{2}$

Eigenvectors: $\frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ i \end{bmatrix} = \frac{1}{\sqrt{2}}\left[\chi_{1/2} + i\chi_{-1/2}\right]$ for $\lambda = \frac{\hbar}{2}$

and $\frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -i \end{bmatrix} = \frac{1}{\sqrt{2}}\left[\chi_{1/2} - i\chi_{-1/2}\right]$ for $\lambda = -\frac{\hbar}{2}$

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- **Pauli Spin Matrices:**

Spin angular momentum can be related with Pauli spin vector as follows:

$$\vec{S} = \frac{\hbar}{2}\vec{\sigma}$$

where $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ are components of the Pauli spin vectors and known as Pauli spin matrices. These matrices satisfies the following conditions:

(i) $\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = I$

(ii) $\sigma_j\sigma_k + \sigma_k\sigma_j = \{\sigma_j, \sigma_k\} = 2I\delta_{jk}$

(iii) $[\sigma_j, \sigma_k] = 2i\,\varepsilon_{jkl}\sigma_l$

(iv) Pauli spin matrices are hermitian, traceless and determinant is -1.

(v) $\sigma_x\sigma_y\sigma_z = iI$

(vi) Since spin does not depend on spatial degrees of freedom then the components of spin S_x, S_y, S_z commute with all spatial operators i.e. momentum, position, orbital angular momentum.

(vii) $e^{i\alpha\sigma_j} = I\cos\alpha + i\sigma_j \sin\alpha$

(viii) For any two vectors $\vec{A}$ and $\vec{B}$, $(\vec{\sigma}.\vec{A})(\vec{\sigma}.\vec{B}) = (\vec{A}.\vec{B})I + i\sigma.(\vec{A}\times\vec{B})$

Example 6. The wave function of an electron at an instant is given by $\psi = f(r,\theta)e^{2i\phi}\chi_{1/2}$. Calculate the average value of z-component of its magnetic moment.

Soln. The operator for the z-component of the magnetic moment is

$$\mu_z = \mu_{Lz} + \mu_{sz} = \frac{\mu_B}{\hbar}L_z + 2\frac{\mu_B}{\hbar}S_z$$

The average value of μ_z in the given state is $\langle\mu_z\rangle = \langle\psi|\mu_z|\psi\rangle$

Now, $\mu_z|\psi\rangle = \frac{\mu_B}{\hbar}\left[L_z|\psi\rangle + 2S_z|\psi\rangle\right]$

The given wave function is $\psi = f(r,\theta)e^{2i\phi}\chi_{1/2}$. The ϕ dependent part is $e^{2i\phi}$. This shows that it is an eigenfunction of L_z with eigenvalue $2\hbar$. The spin dependent part is $\chi_{1/2}$. This shows that it is an eigenfunction of S_z with eigenvalue $+\frac{\hbar}{2}$. Thus

$$L_z|\psi\rangle = 2\hbar|\psi\rangle \text{ and } S_z|\psi\rangle = \frac{\hbar}{2}|\psi\rangle$$

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Therefore, $\mu_z|\psi\rangle = \frac{\mu_B}{\hbar}\left[2\hbar|\psi\rangle + 2\frac{\hbar}{2}|\psi\rangle\right]$

So, $\langle\psi|\mu_z|\psi\rangle = \mu_B\left[2\langle\psi|\psi\rangle + \langle\psi|\psi\rangle\right] = 3\mu_B$

Example 7. The spin part of the wave function of a spin-½ particle is $\cos\alpha\ \chi_{1/2} + \sin\alpha\ e^{i\beta}\chi_{-1/2}$. The x-component of the spin is measured. Find the probability of getting the result $\frac{\hbar}{2}$. Here α and β are real constants.

Soln. The wave function before the measurement is $|\chi_1\rangle = \cos\alpha\,\chi_{1/2} + \sin\alpha\ e^{i\beta}\chi_{-1/2}$.

The wave function after the measurement will be eigenfunction of S_x corresponding to the eigenvalue $\frac{\hbar}{2}$ i.e.

$$|\chi\rangle = \frac{1}{\sqrt{2}}(\chi_{1/2} + \chi_{-1/2})$$

So, probability of getting $\frac{\hbar}{2}$ in a measurement of S_x is $\left|\langle \chi_1 | \chi \rangle\right|^2$

$$\langle \chi_1 | \chi \rangle = \frac{1}{\sqrt{2}}\left\langle \cos\alpha\ \chi_{1/2} + \sin\alpha\ e^{i\beta}\chi_{-1/2} \mid \chi_{1/2} + \chi_{-1/2} \right\rangle$$

$$= \frac{1}{\sqrt{2}}\left[\cos\alpha\langle \chi_{1/2} | \chi_{1/2}\rangle + \sin\alpha\ e^{-i\beta}\langle \chi_{-1/2} | \chi_{-1/2}\rangle\right]$$

$$= \frac{1}{\sqrt{2}}\left(\cos\alpha + \sin\alpha\ e^{-i\beta}\right)$$

Thus the probability is

$$\left|\langle \chi_1 | \chi \rangle\right|^2 = \frac{1}{2}\left(\cos\alpha + \sin\alpha\ e^{-i\beta}\right)\left(\cos\alpha + \sin\alpha\ e^{i\beta}\right)$$

$$= \frac{1}{2}\left[1 + 2\cos\alpha\ \sin\alpha\ \cos\beta\right]$$

Example 8. Find the eigevalue and spin eigenstates of the operator $S_1 = S_x + S_y$

Soln. We know, $S_x = \frac{\hbar}{2}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$ and $S_y = \frac{\hbar}{2}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$

So, $S_1 = S_x + S_y = \frac{\hbar}{2}\begin{bmatrix} 0 & 1-i \\ 1+i & 0 \end{bmatrix}$

Using the standard method of finding eigenvalues and eigenvectors of a matrix, we can get the eigenvalues are

$$\lambda = \pm\frac{\hbar}{\sqrt{2}}$$

The normalized eigenfunction corresponding to $\lambda = \frac{\hbar}{\sqrt{2}}$ will be $\chi_1 = \frac{1}{\sqrt{2}}\chi_{1/2} + \frac{1+i}{2}\chi_{-1/2}$.

The normalized eigenfunction corresponding to $\lambda = \frac{\hbar}{\sqrt{2}}$ will be $\chi_2 = \frac{1}{\sqrt{2}}\chi_{1/2} - \frac{1+i}{2}\chi_{-1/2}$

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Example 9. Calculate $(L_x S_x)\left[Y_1^0(\theta,\phi)\chi_{1/2}\right]$

Soln. $(L_x S_x)\left[Y_1^0(\theta,\phi)\chi_{1/2}\right] = L_x Y_1^0(\theta,\phi) S_x \chi_{1/2}$

$$L_x Y_1^0(\theta,\phi) = \left(\frac{L_+ + L_-}{2}\right)Y_1^0(\theta,\phi) = \frac{1}{2}\left[L_+ Y_1^0(\theta,\phi) + L_- Y_1^0(\theta,\phi)\right]$$

$$= \frac{1}{2}\left[\sqrt{2}\,\hbar Y_1^1(\theta,\phi) + \sqrt{2}\,\hbar Y_1^{-1}(\theta,\phi)\right] = \frac{\hbar}{\sqrt{2}}\left[Y_1^1(\theta,\phi) + Y_1^{-1}(\theta,\phi)\right]$$

and $$S_x\chi_{1/2} = \frac{S_+ + S_-}{2}\chi_{1/2} = \frac{\hbar}{2}\chi_{-1/2}$$

Therefore, $(L_x S_x)\left[Y_1^0(\theta,\phi)_{\chi_{1/2}}\right] = \frac{\hbar^2}{2\sqrt{2}}\left[Y_1^1(\theta,) + Y_1^{-1}(\theta,)\right]\chi_{-1/2}$

Example 10. A particle is in an eigenstate of J_z. Prove that $\langle J_x \rangle = \langle J_y \rangle = 0$. Also find the value of $\langle J_x^2 \rangle$ and $\langle J_y^2 \rangle$.

Soln. Let the eigenstate of J_z be $|jm\rangle$

$$\langle J_x \rangle = \frac{1}{2}\langle jm|(J_+ + J_-)|jm\rangle = \frac{1}{2}\langle jm|J_+|jm\rangle + \frac{1}{2}\langle jm|J_-|jm\rangle$$

$$= \frac{1}{2}\sqrt{j(j+1)-m(m+1)}\,\hbar\langle jm|j,m+1\rangle + \frac{1}{2}\sqrt{j(j+1)-m(m-1)}\,\hbar\langle jm|j,m-1\rangle = 0$$

since $\langle jm|j,m+1\rangle = \langle jm|j,m-1\rangle = 0$.

Similarly, we can get $\langle J_y \rangle = 0$.

We know that, $J_x^2 + J_y^2 = J^2 - J_z^2$

Therefore, $\langle jm|(J_x^2 + J_y^2)|jm\rangle = \langle jm|(J^2 - J_z^2)|jm\rangle$

$$\Rightarrow \langle jm|J_x^2|jm\rangle + \langle jm|J_y^2|jm\rangle = j(j+1)\hbar^2 - m^2\hbar^2$$

It is expected that $\langle J_x^2 \rangle = \langle J_y^2 \rangle$ and, therefore,

$$\langle J_x^2 \rangle = \langle J_y^2 \rangle = \frac{1}{2}[j(j+1)\hbar^2 - m^2\hbar^2]$$

Example 11. The components of arbitrary vectors A and B commute with those of σ. Show that $(\sigma.A)(\sigma.B) = A.B + i\sigma.(A\times B)$.

Soln. $(\sigma.A)(\sigma.B) = (\sigma_x A_x + \sigma_y A_y + \sigma_z A_z)(\sigma_x B_x + \sigma_y B_y + \sigma_z B_z)$

$$= \sigma_x^2 A_x B_x + \sigma_y^2 A_y B_y + \sigma_z^2 A_z B_z + \sigma_x\sigma_y A_x B_y + \sigma_y\sigma_x A_y B_x$$
$$+ \sigma_x\sigma_z A_x B_z + \sigma_y\sigma_z A_y B_z + \sigma_z\sigma_y A_z B_y + \sigma_z\sigma_x A_z B_x$$

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Using the relations $\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = 1$, $\sigma_x\sigma_y = i\sigma_z$, $\sigma_y\sigma_z = i\sigma_x$, $\sigma_z\sigma_x = i\sigma_y$,

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$\sigma_x\sigma_y + \sigma_y\sigma_x = \sigma_y\sigma_z + \sigma_z\sigma_y = \sigma_z\sigma_x + \sigma_x\sigma_z = 0$

We get $(\sigma.A)(\sigma.B) = (A.B) + i\sigma_z(A_xB_y - A_yB_x) + i\sigma_y(A_zB_x - A_xB_z) + i\sigma_x(A_yB_z - A_zB_y)$

$$= (A.B) + i\sigma.(A\times B)$$

Example 12. Find the equivalence of the following operators:

(i) $S_x^2 S_y S_z^2$; (ii) $S_x^2 S_y^2 S_z^2$; (iii) $S_x S_y S_z^3$

Soln. (i) $S_x^2 S_y S_z^2 = \left(\frac{\hbar}{2}\right)^2 \sigma_x^2 \frac{\hbar}{2}\sigma_y \left(\frac{\hbar}{2}\right)^2 \sigma_z^2 = \left(\frac{\hbar}{2}\right)^5 \sigma_y$

(ii) $S_x^2 S_y^2 S_z^2 = \left(\frac{\hbar}{2}\right)^2 \sigma_x^2 \left(\frac{\hbar}{2}\right)^2 \sigma_y^2 \left(\frac{\hbar}{2}\right)^2 \sigma_z^2 = \left(\frac{\hbar}{2}\right)^6$

(iii) $S_x S_y S_z^3 = \frac{\hbar}{2}\sigma_x \frac{\hbar}{2}\sigma_y \left(\frac{\hbar}{2}\right)^3 \sigma_x^3 = \left(\frac{\hbar}{2}\right)^5 \sigma_x\sigma_y\sigma_z = \left(\frac{\hbar}{2}\right)^5 i$.

Example 13. Consider a spin (1/2) particle of mass m with charge $-e$ in an external magnetic field B.
(i) What is the Hamiltonian of the system?
(ii) If S is the spin angular momentum vector, show that

$$\frac{dS}{dt} = -\frac{e}{m}(S \times B)$$

Soln. (i) The magnetic dipole moment of the particle is $\vec{\mu} = -g_s \frac{e}{2m}\vec{S} = -\frac{e}{m}\vec{S}$

The interaction energy E of the dipole moment μ in an external magnetic field B is given by

$$E = -\vec{\mu}.\vec{B} = \frac{e}{m}\vec{S}.\vec{B}$$

The corresponding Hamiltonian will be $\left[\vec{S}, S_x B_x\right] = B_x\left(-i\hbar S_y\hat{i} + i\hbar S_z\hat{j}\right)$

(ii) In the Heisenberg picture,

$$\frac{d\vec{S}}{dt} = \left[\vec{S}, S_x B_x\right] + \left[\vec{S}, S_y B_y\right] + \left[\vec{S}, S_z B_z\right]$$

$$= \frac{e}{i\hbar m}(-i\hbar)\left[\left(S_y B_z - S_z B_y\right)\hat{i} + \left(B_x S_z - B_z S_x\right)\hat{j} + \left(S_x B_y - B_y S_x\right)\hat{k}\right]$$

$$= -\frac{e}{m}\left(\vec{S} \times \vec{B}\right)$$

$$= \frac{e}{i\hbar m}[S, S_x B_x + S_y B_y + S_z B_z]$$

$$\left[\vec{S}, S_x B_x\right] = B_x\left[\vec{S}, S_x\right] = B_x\left[S_x, S_x\right]\hat{i} + B_x\left[S_y, S_x\right]\hat{j} + B_x\left[S_z, S_x\right]\hat{k}$$

$$= B_x\left(-i\hbar S_z\hat{j} + i\hbar S_y\hat{k}\right)$$

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Similarly, $\left[\vec{S}, S_y B_y\right] = B_y\left(i\hbar S_z\hat{i} - i\hbar S_x\hat{k}\right)$

and $\left[\vec{S}, S_z B_z\right] = B_z\left(-i\hbar S_y\hat{i} + i\hbar S_x\hat{j}\right)$

Therefore, $\frac{d\vec{S}}{dt} = \left[\vec{S}, S_x B_x\right] + \left[\vec{S}, S_y B_y\right] + \left[\vec{S}, S_z B_z\right]$

$$= \frac{e}{i\hbar m}(-i\hbar)\left[\left(S_y B_z - S_z B_y\right)\hat{i} + \left(B_x S_z - B_z S_x\right)\hat{j} + \left(S_x B_y - B_y S_x\right)\hat{k}\right]$$

$$= -\frac{e}{m}\left(\vec{S} \times \vec{B}\right)$$

Example 14. Consider a system of two spin-half particles, in a state with total spin quantum number S = 0. Find the eigenvalue of the spin Hamiltonian $H = A S_1.S_2$, where A is a positive constant in this state.

Soln. The total spin angular momentum S of the two-spin system is given by

Eigenvalue of $AS_1.S_2 = A\left[\dfrac{s(s+1)\hbar^2 - s_1(s_1+1)\hbar^2 - s_2(s_2+1)\hbar^2}{2}\right]$

$$= A\left[\frac{0-(3/4)\hbar^2-(3/4)\hbar^2}{2}\right] = -\frac{3}{4}A\hbar^2$$

Example 15. An operator P describing the interaction of two spin-half particles is $P = a + b\sigma_1.\sigma_2$, where a, b are constants, with σ_1 and σ_2 being the Pauli matrices of the two spins. The total spin angular momentum $S = S_1 + S_2 = (1/2)\hbar(\sigma_1 + \sigma_2)$. Show that P, S^2 and S_z can be measured simultaneously.

Soln. P, S^2 and S_z can be measured simultaneously if

$$[P, S^2] = [P, S_z] = [S^2, S_z] = 0$$

We know that $[S^2, S_z] = 0$. From the definition

$$S^2 = \frac{\hbar^2}{4}(\sigma_1^2 + \sigma_1^2 + 2\vec{\sigma}_1.\vec{\sigma}_2) \Rightarrow \vec{\sigma}_1.\vec{\sigma}_2 = \frac{2S^2}{\hbar^2} - \frac{1}{2}(\sigma_1^2 + \sigma_2^2)$$

Since for each particle $\vec{\sigma}^2 = \sigma_x^2 + \sigma_y^2 + \sigma_z^2 = 3I$, where I is the unit matrix,

Therefore, $\sigma_1.\sigma_1 = \dfrac{2S^2}{\hbar^2} - 3I$

Now, $[S^2, P] = [S^2, a] + b[S^2, \sigma_1.\sigma_2] = b\left[S^2, \dfrac{2S^2}{\hbar^2} - 3I\right] = b\left[S^2, \dfrac{2S^2}{\hbar^2}\right] - b[S^2, 3I] = 0$

and $[S_z, P] = [S_z, a] + b\left[S_z, \dfrac{2S^2}{\hbar^2} - 3I\right] = 0$

Since S^2 and S_z commute with P, all the three can be measured simultaneously.

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Example 16. Obtain the Hamiltonian operator for a free electron having magnetic moment μ in an external magnetic field B_z in the z-direction in the electron's reference frame. If another constant magnetic field B_y is applied in the y-direction, obtain the time rate of change of μ in the Heisenberg picture.

Soln. The magnetic moment of the electron is given by

$$\vec{\mu} = -\frac{e}{m}\vec{S} = -\frac{e\hbar}{2m}\vec{\sigma} = -\mu_B\vec{\sigma}$$

The Hamiltonian

$$H' = -\vec{\mu}.\vec{B} = -\mu_z B_z = \mu_B \sigma_z B_z$$

For total applied magnetic field $B = B_y\hat{y} + B_z\hat{z}$, the total Hamiltonian

$$H = \mu_B(\sigma_z B_z + \sigma_y B_y)$$

From equation

$$\frac{d\mu}{dt} = \frac{1}{i\hbar}[\mu, H] = \frac{1}{i\hbar}[-\mu_B\sigma, \mu_B(\sigma_z B_z + \sigma_y B_y)]$$

$$= -\frac{\mu_B^2}{i\hbar}[\sigma_x\hat{x} + \sigma_y\hat{y} + \sigma_z\hat{z}, \sigma_z B_z + \sigma_y B_y]$$

$$= -\frac{\mu_B^2}{i\hbar}[\sigma_x, \sigma_z]B_z\hat{x} + [\sigma_x, \sigma_y]B_y\hat{x} + [\sigma_y, \sigma_z]B_z\hat{y} + [\sigma_y, \sigma_y]B_y\hat{y} + [\sigma_z, \sigma_z]B_z\hat{z} + [\sigma_z, \sigma_y]B_y\hat{z}$$

Using the commutation relations among $\sigma_x, \sigma_y, \sigma_z$, we get

$$\frac{d\mu}{dt} = \frac{i}{\hbar}\mu_B^2[-2i\sigma_y B_z\hat{x} + 2i\sigma_z B_y\hat{x} + 2i\sigma_x B_z\hat{y} - 2i\sigma_x B_y\hat{z}]$$

$$= \frac{2}{\hbar}\mu_B^2[(\sigma_y B_z - \sigma_z B_y)\hat{x} - \sigma_x B_z\hat{y} + \sigma_x B_y\hat{z}]$$

$$= \frac{2}{\hbar}\mu_B^2[\sigma \times B] = -\frac{2}{\hbar}\mu_B^2[B \times \sigma] \quad = \frac{e}{m}[B \times \mu]$$

which is the time rate of change of the magnetic moment.

Example 17. The state of the hydrogen atom is $2p$ state. Find the energy levels of the spin-orbit interaction Hamiltonian $A\vec{L}.\vec{S}$, where A is a constant.

Soln. The $2p$ state means $s = 1/2, l = 1$ and $j = \frac{1}{2}, \frac{3}{2}$. The total angular momentum

$$H = AL.S = \frac{A}{2}\left(J^2 - L^2 - S^2\right)$$

Therefore, the corresponding energy levels will be

$$E = \frac{A}{2}\left[j(j+1)\hbar^2 - l(l+1)\hbar^2 - s(s+1)\hbar^2\right]$$

Using equation (ii)-(v), the energy eigenvalue of H_{so} is given by

For $j = \frac{3}{2}, E = \frac{A}{2}\left[\frac{15}{4}\hbar^2 - 2\hbar^2 - \frac{3}{4}\hbar^2\right] = \frac{A}{2}\hbar^2$

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For $j = \frac{1}{2}, E_{so} = \frac{A}{2}\left[\frac{3}{4}\hbar^2 - 2\hbar^2 - \frac{3}{4}\hbar^2\right] = -A\hbar^2$

Example 18. The Hamiltonian of a system of 3 non-identical spin-half particles is

$$H = AS_1.S_2 - B(S_1 + S_2).S_3$$

where A and B are constants are S_1, S_2 and S_3 are the spin angular momentum operators. Find their energy levels and their degeneracies.

Soln. Writing $S = S_1 + S_2 + S_3$ and $S_{12} = S_1 + S_2$, we have

$$S^2 = S_{12}^2 + S_3^2 + 2S_{12}.S_3 \Rightarrow S_{12}.S_3 = \frac{1}{2}(S^2 - S_{12}^2 - S_3^2)$$

Similarly, $S_1.S_2 = \frac{1}{2}(S_{12}^2 - S_1^2 - S_2^2)$

since $s_1 = 1/2$ and $s_2 = 1/2$, the possible values of the quantum number $s_{12} = 0$ and 1.

When $s_{12} = 0$, the possible values of $S = 1/2$ and $1/3$. The Hamiltonian becomes

$$H = AS_1.S_2 - B(S_1 + S_2).S_3$$

$$= \frac{A}{2}(S_{12}^2 - S_1^2 - S_2^2) + \frac{B}{2}(S^2 - S_{12}^2 - S_3^2)$$

The energy is

$$E = \frac{A}{2}\hbar^2[s_{12}(s_{12}+1) - s_1(s_1+1) - s_2(s_2+1)] + \frac{B}{2}\hbar^2[s(s+1) - s_{12}(s_{12}+1) - s_3(s_3+1)]$$

Since $s_1 = s_2 = s_3 = 1/2$,

$$E_{s_{12},s} = \frac{A}{2}\hbar^2\left[s_{12}(s_{12}+1) - \frac{3}{2}\right] + \frac{B}{2}\hbar^2\left[s(s+1) - s_{12}(s_{12}+1) - \frac{3}{4}\right]$$

As $s = 1/2$ when $s_{12} = 0$, $E_{0,1/2} = -\frac{3}{4}\hbar^2$ which is $2s + 1 = 2$-fold degenerate.

As $s = 1/2$ and $3/2$, when $s_{12} = 1$,

$$E_{1,1/2} = \frac{A}{4}\hbar^2\left(2 - \frac{3}{2}\right) + \frac{B}{4}\hbar^2\left(\frac{3}{4} - 2 - \frac{3}{4}\right) = \frac{A}{4}\hbar^2 - B\hbar^2 = \left(\frac{A}{4} - B\right)\hbar^2$$

which is $2s + 1 = 2$-fold degenerate.

$$E_{1,3/2} = \frac{A}{2}\hbar^2\left(2 - \frac{3}{2}\right) + \frac{B}{2}\hbar^2\left(\frac{15}{4} - 2 - \frac{3}{4}\right) = \left(\frac{A}{4} + \frac{B}{2}\right)\hbar^2$$

which is $2s + 1 = 4$ fold degenerate.

Example 19. The two spin-half particles are described by the Hamiltonian

$$H = A(S_{1z} + S_{2z}) + B(S_1.S_2)$$

where A and B are constants and S_1 and S_2 are the spin angular momenta of the two spins. Find the energy levels of the system.

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Soln. Total spin angular momentum $S = S_1 + S_2$, $S_z = S_{1z} + S_{2z}$

$$S_1.S_2 = \frac{1}{2}(S^2 - S_1^2 - S_2^2)$$

Since $s_1 = 1/2$ and $s_2 = 1/2$, the possible values of s are 0 and 1.

The Hamiltonian, $H = A(S_{1z} + S_{2z}) + B(S_1.S_2) = AS_z + \frac{B}{2}(S^2 - S_1^2 - S_2^2)$

The corresponding energy will be

$$E_{s,M_s} = Am_s\hbar + \frac{B}{2}\hbar^2\left[s(s+1) - \frac{3}{4} - \frac{3}{4}\right]$$

When $s = 0$, the possible values of $m_s = 0$, then $E_{0,0} = -\frac{3}{4}B\hbar^2$,

When s = 1, the possible values of $m_s = 1, 0, -1$, then $E_{1,1} = A\hbar + \frac{B}{4}\hbar^2$

Example 20. For a spin 1/2 particle, the expectation value of $S_xS_yS_z$ is

(a) $\frac{i\hbar^3}{8}$ (b) $-\frac{i\hbar^3}{8}$ (c) $\frac{i\hbar^3}{16}$ (d) $-\frac{i\hbar^3}{16}$

Soln. $S_xS_yS_z = \frac{\hbar^3}{8}\sigma_x\sigma_y\sigma_z = \frac{\hbar^3}{8}\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}\begin{bmatrix}0 & -i\\ i & 0\end{bmatrix}\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix} = \frac{i\hbar^3}{8}\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}$

$\langle S_xS_yS_z\rangle = \langle\psi|S_xS_yS_z|\psi\rangle$

$= \frac{i\hbar^3}{8}\begin{bmatrix}a^* & b^*\end{bmatrix}\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}\begin{bmatrix}a\\ b\end{bmatrix} = \frac{i\hbar^3}{8}\left[a^*a + b^*b\right] = \frac{i\hbar^3}{8}$

Example 21. A spin ½ particle is in the state $S_z = \frac{\hbar}{2}$. The expectation value of S_x, S_x^2, S_y, S_y^2 are

(a) $0, 0, \frac{\hbar^2}{4}, \frac{\hbar^2}{4}$ (b) $\frac{\hbar^2}{4}, 0, \frac{\hbar^2}{4}, 0$ (c) $0, \frac{\hbar^2}{4}, 0, \frac{\hbar^2}{4}$ (d) $\frac{\hbar^2}{4}, \frac{\hbar^2}{4}, 0, 0$

Soln. Eigenstate corresponding, $S = \frac{\hbar}{2}$ is $\begin{bmatrix}1\\ 0\end{bmatrix}$

$\langle S_x\rangle = \langle\psi|S_x|\psi\rangle = \begin{bmatrix}1 & 0\end{bmatrix}\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}\begin{bmatrix}1\\ 0\end{bmatrix}\frac{\hbar}{2} = \frac{\hbar}{2}\begin{bmatrix}1 & 0\end{bmatrix}\begin{bmatrix}0\\ 1\end{bmatrix} = 0$

$\langle S_y\rangle = \langle\psi|S_y|\psi\rangle = 0$

$\langle S_x^2\rangle = \langle\psi|S_x^2|\psi\rangle = \frac{\hbar^2}{4}\begin{bmatrix}1 & 0\end{bmatrix}\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}\begin{bmatrix}1\\ 0\end{bmatrix} = \frac{\hbar^2}{4}$

$\langle S_y^2\rangle = \langle\psi|S_y^2|\psi\rangle = \frac{\hbar^2}{4}$

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Example 22. An electron is in the state with spin wave function, $\phi_s = \begin{bmatrix}\sqrt{3}/2\\ 1/2\end{bmatrix}$ is in S_z representation.

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What is the probability of finding the z-component of its spin along the z-direction?

Soln. $\phi_s = \begin{bmatrix}\sqrt{3}/2\\ 1/2\end{bmatrix} = c_1\underset{\text{along } +z}{\begin{bmatrix}1\\ 0\end{bmatrix}} + c_2\underset{\text{along } -z}{\begin{bmatrix}0\\ 1\end{bmatrix}} \quad \Rightarrow c_1 = \frac{\sqrt{3}}{2},\ c_2 = \frac{1}{2}$

Probability of finding z-components of its spin in –z direction $= \frac{1}{4}$

Example 23. Suppose a spin ½ particle is in the state $|\phi\rangle = \frac{1}{\sqrt{6}}\begin{bmatrix}1+i\\ 2\end{bmatrix}$

What are probabilities of getting $+\frac{\hbar}{2}$ and $-\frac{\hbar}{2}$ if

(i) z component of spin is measured?

(ii) x component of spin is measured?

(iii) calculate the expectation value of S_x i.e. $\langle S_x \rangle$

Soln. (i) Given: $|\phi\rangle = \frac{1}{\sqrt{6}}\begin{bmatrix}1+i\\2\end{bmatrix} = c_1\begin{bmatrix}1\\0\end{bmatrix} + c_2\begin{bmatrix}0\\1\end{bmatrix} \quad \Rightarrow c_1 = \frac{1+i}{\sqrt{6}}, c_2 = \frac{2}{\sqrt{6}}$

Probability of getting $S_z = \frac{\hbar}{2}$ is $\left|\frac{1}{\sqrt{6}}(1+i)\right|^2 = \frac{2}{6} = \frac{1}{3}$

Probability of getting $S_z = -\frac{\hbar}{2}$ is $\left|\frac{2}{\sqrt{6}}\right|^2 = \frac{4}{6} = \frac{2}{3}$

(ii) Given: $|\phi\rangle = \frac{1}{\sqrt{6}}\begin{bmatrix}1+i\\2\end{bmatrix} = \frac{c_1}{\sqrt{2}}\begin{bmatrix}1\\1\end{bmatrix} + \frac{c_2}{\sqrt{2}}\begin{bmatrix}1\\-1\end{bmatrix}$

$\Rightarrow \quad c_1 = \frac{1}{\sqrt{2}}\left(\frac{3+i}{\sqrt{6}}\right), c_2 = \frac{1}{\sqrt{2}}\left(\frac{-1+i}{\sqrt{6}}\right)$

Probability of getting $S_x = \frac{\hbar}{2}$ is $\frac{5}{6}$

Probability of getting $S_x = -\frac{\hbar}{2}$ is $\frac{1}{6}$

(iii) $\langle S_x \rangle = P_1(S_x)_1 + P_2(S_x)_2 = \frac{5}{6}\times\frac{\hbar}{2} - \frac{1}{6}\times\frac{\hbar}{2} = \frac{\hbar}{3}$

CSIR PREVIOUS YEAR QUESTIONS

1. The Hamiltonian of an electron in a constant magnetic field $\vec{B}$ is given by $H = \mu\vec{\sigma}.\vec{B}$ where μ is a positive constant and $\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ denotes the Pauli matrices. Let $\omega = \mu B/\hbar$ and I be the 2×2 unit matrix. Then the operator $e^{iHt/\hbar}$ simplifies to **[CSIR June 2011]**

(a) $I\cos\frac{\omega t}{2} + \frac{i\vec{\sigma}.\vec{B}}{B}\sin\frac{\omega t}{2}$ (b) $I\cos\omega t + \frac{i\vec{\sigma}.\vec{B}}{B}\sin\omega t$

(c) $I\sin\omega t + \frac{i\vec{\sigma}.\vec{B}}{B}\cos\omega t$ (d) $I\sin 2\omega t + \frac{i\vec{\sigma}.\vec{B}}{B}\cos 2\omega t$

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Soln. Given operator: $e^{i\frac{H}{\hbar}t} = e^{i\mu\frac{\vec{\sigma}.\vec{B}}{\hbar}t} = e^{i\frac{\mu Bt}{\hbar}(\vec{\sigma}.\hat{B})} = e^{i\omega t(\vec{\sigma}.\hat{B})}$

Using the identity, $e^{i\theta\vec{\sigma}.\hat{n}} = I\cos\theta + i\vec{\sigma}.\hat{n}\sin\theta$ (where $\hat{n}$ is unit vector), we get

$$e^{i\frac{H}{\hbar}t} = e^{i\omega t(\vec{\sigma}.\hat{B})} = I\cos\omega t + i\vec{\sigma}.\hat{B}\sin\omega t = I\cos\omega t + i\frac{\vec{\sigma}.B}{B}\sin\omega t$$

Correct option is (b)

2. In a system consisting of two spin $\frac{1}{2}$ particles labeled 1 and 2, let $\vec{S}^{(1)} = \frac{\hbar}{2}\vec{\sigma}^{(1)}$ and $\vec{S}^{(2)} = \frac{\hbar}{2}\vec{\sigma}^{(2)}$ denote the corresponding spin operators. Here $\vec{\sigma} \equiv (\sigma_x, \sigma_y, \sigma_z)$ and $\sigma_x, \sigma_y, \sigma_z$ are the three Pauli matrices.

[CSIR June 2011]

A. In the standard basis the matrices for the operators $S_x^{(1)} S_y^{(2)}$ and $S_y^{(1)} S_x^{(2)}$ respectively,

(a) $\frac{\hbar^2}{4}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}, \frac{\hbar^2}{4}\begin{pmatrix}-1 & 0\\ 0 & 1\end{pmatrix}$ (b) $\frac{\hbar^2}{4}\begin{pmatrix}i & 0\\ 0 & -i\end{pmatrix}, \frac{\hbar^2}{4}\begin{pmatrix}-i & 0\\ 0 & i\end{pmatrix}$

(c) $\frac{\hbar^2}{4}\begin{pmatrix}0 & 0 & 0 & -i\\ 0 & 0 & i & 0\\ 0 & -i & 0 & 0\\ i & 0 & 0 & 0\end{pmatrix}, \frac{\hbar^2}{4}\begin{pmatrix}0 & 0 & 0 & -i\\ 0 & 0 & -i & 0\\ 0 & i & 0 & 0\\ i & 0 & 0 & 0\end{pmatrix}$ (d) $\frac{\hbar^2}{4}\begin{pmatrix}0 & 1 & 0 & 0\\ 1 & 0 & 0 & 0\\ 0 & 0 & 0 & -i\\ 0 & 0 & i & 0\end{pmatrix}, \frac{\hbar^2}{4}\begin{pmatrix}0 & -i & 0 & 0\\ i & 0 & 0 & 0\\ 0 & 0 & 0 & 1\\ 0 & 0 & 1 & 0\end{pmatrix}$

B. These two operators satisfy the relation

(a) $\left\{S_x^{(1)}S_y^{(2)}, S_y^{(1)}S_x^{(2)}\right\} = S_z^{(1)}S_z^{(2)}$ (b) $\left\{S_x^{(1)}S_y^{(2)}, S_y^{(1)}S_x^{(2)}\right\} = 0$

(c) $\left[S_x^{(1)}S_y^{(2)}, S_y^{(1)}S_x^{(2)}\right] = S_z^{(1)}S_z^{(2)}$ (d) $\left[S_x^{(1)}S_y^{(2)}, S_y^{(1)}S_x^{(2)}\right] = 0$

Soln. **A.** Pauli Spin matrices:

$$\sigma_x = \frac{\hbar}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}, \sigma_y = \frac{\hbar}{2}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}, \sigma_z = \frac{\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$$

$$S_x^{(1)}S_y^{(2)} = \frac{\hbar^2}{4}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix} = \frac{\hbar^2}{4}\begin{pmatrix}0 & 0 & 0 & -i\\ 0 & 0 & i & 0\\ 0 & -i & 0 & 0\\ i & 0 & 0 & 0\end{pmatrix}$$

$$S_y^{(1)}S_x^{(2)} = \frac{\hbar^2}{4}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} = \frac{\hbar^2}{4}\begin{pmatrix}0 & 0 & 0 & -i\\ 0 & 0 & -i & 0\\ 0 & i & 0 & 0\\ i & 0 & 0 & 0\end{pmatrix}$$

Correct answer is (c)

B. $\left[S_x^{(1)}S_y^{(2)}, S_y^{(1)}S_x^{(2)}\right] = S_x^{(1)}S_y^{(2)}S_y^{(1)}S_x^{(2)} - S_y^{(1)}S_x^{(2)}S_x^{(1)}S_y^{(2)}$

$$= \frac{\hbar^2}{4}\begin{pmatrix}0 & 0 & 0 & -i\\ 0 & 0 & i & 0\\ 0 & -i & 0 & 0\\ i & 0 & 0 & 0\end{pmatrix}\frac{\hbar^2}{4}\begin{pmatrix}0 & 0 & 0 & -i\\ 0 & 0 & -i & 0\\ 0 & i & 0 & 0\\ i & 0 & 0 & 0\end{pmatrix} - \frac{\hbar^2}{4}\begin{pmatrix}0 & 0 & 0 & -i\\ 0 & 0 & -i & 0\\ 0 & i & 0 & 0\\ i & 0 & 0 & 0\end{pmatrix}\frac{\hbar^2}{4}\begin{pmatrix}0 & 0 & 0 & -i\\ 0 & 0 & i & 0\\ 0 & -i & 0 & 0\\ i & 0 & 0 & 0\end{pmatrix} = 0$$

Correct answer is (d)

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3. In a basis in which the z-component S_z of the spin is diagonal, an electron is in a spin state

$$\psi = \begin{pmatrix} (1+i)/\sqrt{6} \\ \sqrt{2/3} \end{pmatrix}$$

The probabilities that a measurement of S_z will yield the values $\hbar/2$ and $-\hbar/2$ are, respectively **[CSIR June 2013]**

(a) 1/2 and 1/2 (b) 2/3 and 1/3 (c) 1/4 and 3/4 (d) 1/3 and 2/3

Soln. The eigenfunctions of S_z in a basis in which S_z is diagonal are

$$|\phi_1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \text{ for } \frac{\hbar}{2} \text{ eigenvalue}$$

and $$|\phi_2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \text{ for } -\frac{\hbar}{2} \text{ eigenvalue}$$

The given state can be written as linear superposition of $|\phi_1\rangle$ and $|\phi_2\rangle$ as

$$\begin{pmatrix} (1+i)/\sqrt{6} \\ \sqrt{\frac{2}{3}} \end{pmatrix} = c_1 \begin{pmatrix} 1 \\ 0 \end{pmatrix} + c_2 \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{(1+i)}{\sqrt{6}} \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \sqrt{\frac{2}{3}} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

The probability of yielding the value $+\frac{\hbar}{2}$

$$= \left|\frac{1-i}{\sqrt{6}}\right|^2 = \frac{(1+i)(1-i)}{6} = \frac{2}{6} = \frac{1}{3}$$

and the probability of yielding the value $-\frac{\hbar}{2} = \left|\sqrt{\frac{2}{3}}\right|^2 = \frac{2}{3}$

Correct answer is (d)

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4. A spin $-\frac{1}{2}$ particle is in the state $\chi = \frac{1}{\sqrt{11}}\begin{pmatrix} 1+i \\ 3 \end{pmatrix}$ in the eigenbasis of S^2 and S_z. If we measure S_z the

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probabilities of getting $+\frac{\hbar}{2}$ and $-\frac{\hbar}{2}$, respectively, are **[CSIR Dec 2013]**

(a) $\frac{1}{2}$ and $\frac{1}{2}$ (b) $\frac{2}{11}$ and $\frac{9}{11}$ (c) 0 and 1 (d) $\frac{1}{11}$ and $\frac{3}{11}$

Soln. Given : A spin $\frac{1}{2}$ particle is in the state $\chi = \frac{1}{\sqrt{11}}\begin{pmatrix} 1+i \\ 3 \end{pmatrix}$

Measurement of S_z gives $+\frac{\hbar}{2}$ and $-\frac{\hbar}{2}$ with respective eigenbasis $\chi_{1/2} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ and $\chi_{-1/2} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$

Method-1:

$$\frac{1}{\sqrt{11}}\begin{pmatrix} 1+i \\ 3 \end{pmatrix} = C_1 \begin{bmatrix} 1 \\ 0 \end{bmatrix} + C_2 \begin{bmatrix} 0 \\ 1 \end{bmatrix} \quad C_1 = \frac{1+i}{\sqrt{11}} \quad C_2 = \frac{3}{\sqrt{11}}$$

Probability of finding S_z as $+\frac{\hbar}{2}$ and $-\frac{\hbar}{2}$ are $|C_1|^2 = \frac{2}{11}$ and $|C_2|^2 = \frac{9}{11}$ respectively.

Method-2:

Initial state of particle = $|\psi_i\rangle = \frac{1}{\sqrt{11}}\begin{pmatrix} 1+i \\ 3 \end{pmatrix}$

Final state of particle = $|\psi_{f_1}\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ and $|\psi_{f_2}\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$

Probability of finding S_z as $+\frac{\hbar}{2}$ and $-\frac{\hbar}{2}$ are $|\langle\psi_{f_1}|\psi_i\rangle|^2 = \frac{2}{11}$ and $|\langle\psi_{f_2}|\psi_i\rangle|^2 = \frac{9}{11}$ respectively.

Correct answer is (b)

5. Let ψ_{nlm} denote the eigenfunctions of a Hamiltonian for a spherically symmetric potential $V(r)$. The expectation value of L_z in the state

$\psi = \frac{1}{6}\left[\psi_{200} + \sqrt{5}\,\psi_{210} + \sqrt{10}\,\psi_{21-1} + \sqrt{20}\,\psi_{211}\right]$ is **[CSIR Dec 2013]**

(a) $-\frac{5}{18}\hbar$ (b) $\frac{5}{6}\hbar$ (c) $\hbar$ (d) $\frac{5}{18}\hbar$

Soln. Given: $\psi = \frac{1}{6}\left[\psi_{200} + \sqrt{5}\,\psi_{2100} + \sqrt{10}\,\psi_{21-1} + \sqrt{20}\psi_{211}\right]$

Since, $\hat{L}_z\psi_{n\ell m} = m\hbar\psi_{n\ell m}$

Therefore, $\langle L_z\rangle = \sum_i P_i(L_z)_i = \frac{1}{36}(0) + \frac{5}{36}(0) + \frac{10}{36}(-\hbar) + \frac{20}{36}(\hbar) \Rightarrow \langle L_z\rangle = \frac{5}{16}\hbar$

Correct answer is (d)

6. The expectation value of the x-component of the orbital angular momentum L_x in the state

$\psi = \frac{1}{5}\left[3\psi_{2,1,-1} + \sqrt{5}\psi_{2,1,0} - \sqrt{11}\psi_{2,1,+1}\right]$ (where ψ_{lm} are the eigenfunctions in usual notation), is

[CSIR Dec 2013]

(a) $-\frac{\hbar\sqrt{10}}{25}(\sqrt{11}-3)$ (b) 0

(c) $\frac{\hbar\sqrt{10}}{25}(\sqrt{11}+3)$ (d) $\hbar\sqrt{2}$

Soln. Given : $\psi = \frac{1}{5}\left[3\psi_{2,1,-1} + \sqrt{5}\,\psi_{2,1,0} - \sqrt{11}\psi_{2,1,+1}\right]$

$\langle L_x\rangle = \langle\psi|L_x|\psi\rangle$

$= \frac{1}{5}\left[3\langle\psi_{2,1,-1}| + \sqrt{5}\langle\psi_{2,1,0}| - \sqrt{11}\langle\psi_{2,1,1}|\right]\left[\frac{1}{2}(L_+ + L_-)\right]$

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$$\left[\frac{3}{5}\left|\psi_{2,1,-1}\right\rangle+\frac{\sqrt{5}}{5}\left|\psi_{2,1,0}\right\rangle-\frac{\sqrt{11}}{5}\left|\psi_{2,1,1}\right\rangle\right]$$

Now, we know, $\hat{L}_+\psi_{n\ell m}=\sqrt{(\ell-m)(\ell+m+1)}\,\hbar\psi_{n\ell m+1}$

$$\hat{L}_-\psi_{n\ell m}=\sqrt{(\ell+m)(\ell-m+1)}\hbar\psi_{n\ell m-1}$$

$$\Rightarrow \quad \langle L_x\rangle=\left[\frac{3}{5}\left\langle\psi_{2,1,-1}\right|+\frac{\sqrt{5}}{5}\left\langle\psi_{2,1,0}\right|-\frac{\sqrt{11}}{5}\left\langle\psi_{2,1,1}\right|\right]$$

$$\frac{1}{2}\left[\frac{3}{5}\sqrt{2}\,\hbar\left|\psi_{2,1,0}\right\rangle+\frac{\sqrt{5}}{5}\sqrt{2}\,\hbar\left|\psi_{2,1,1}\right\rangle+\frac{\sqrt{5}}{5}\sqrt{2}\hbar\left|\psi_{2,1,-1}\right\rangle-\frac{\sqrt{11}}{5}\sqrt{2}\hbar\left|\psi_{2,1,0}\right\rangle\right]$$

$$\Rightarrow \quad \langle L_x\rangle=\frac{1}{2}\frac{\sqrt{5}}{5}.\sqrt{2}\hbar\left(\frac{3}{5}-\frac{\sqrt{11}}{5}\right)+\frac{1}{2}.\frac{3}{5}.\frac{\sqrt{5}}{5}\sqrt{2}\hbar-\frac{\sqrt{11}}{5}.\frac{1}{2}.\frac{\sqrt{5}}{5}\sqrt{2}\hbar$$

$$=\frac{3\sqrt{5}}{25}\sqrt{2}\hbar-\frac{\sqrt{11}\sqrt{5}}{25}\sqrt{2}\hbar=-\frac{\hbar\sqrt{10}}{25}\left(\sqrt{11}-3\right)$$

Correct answer is (a)

7. A particle is prepared in a simultaneous eigenstate of L^2 and L_z. If $\ell(\ell+1)\hbar^2$ and $m\hbar$ are respectively the eigenvalues of L^2 and L_z, then the expectation value $\langle L_x^2\rangle$ of the particle in this state satisfies

[CSIR Dec 2013]

(a) $\langle L_x^2\rangle=0$ (b) $0\le\langle L_x^2\rangle\le\ell^2\hbar^2$

(c) $0\le\langle L_x^2\rangle\le\frac{\ell(\ell+1)\hbar^2}{3}$ (d) $\frac{\ell\hbar^2}{2}\le\langle L_x^2\rangle\le\frac{\ell(\ell+1)\hbar^2}{2}$

Soln. $\left\langle\hat{L}_x^2+\hat{L}_y^2\right\rangle=\left\langle\hat{L}^2\right\rangle-\left\langle\hat{L}_z^2\right\rangle=\ell(\ell+1)\hbar^2-m^2\hbar^2$

Since, $\left\langle\hat{L}_x^2\right\rangle=\left\langle\hat{L}_y^2\right\rangle$ then $\left\langle\hat{L}_x^2\right\rangle=\frac{1}{2}\left[\ell(\ell+1)\hbar^2-m^2\hbar^2\right]$

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For a given l, m varies from $-l$ to l.

$\left\langle\hat{L}_x^2\right\rangle_{\max}$ occurs when $m=0$ $\Rightarrow$ $\left\langle\hat{L}_x^2\right\rangle_{\max}=\frac{1}{2}\ell(\ell+1)\hbar^2$

$\left\langle\hat{L}_x^2\right\rangle_{\min}$ occurs when $m=\pm\ell$ $\Rightarrow$ $\left\langle\hat{L}_x^2\right\rangle_{\min}=\frac{1}{2}\ell\hbar^2$

Correct answer is (d)

8. Consider the normalized wavefunction $\phi=a_1\psi_{11}+a_2\psi_{10}+a_3\psi_{1-1}$ where ψ_{lm} is a simultaneous normalized eigenfunction of the angular momentum operators L^2 and L_z, with eigenvalues $l(l+1)\hbar^2$ and $m\hbar$ respectively. If ϕ is an eigenfunction of the operator L_x with eigenvalue $\hbar$, then

[CSIR Dec 2014]

(a) $a_1 = -a_3 = \frac{1}{2}, a_2 = \frac{1}{\sqrt{2}}$ (b) $a_1 = a_3 = \frac{1}{2}, a_2 = \frac{1}{\sqrt{2}}$

(c) $a_1 = a_3 = \frac{1}{2}, a_2 = -\frac{1}{\sqrt{2}}$ (d) $a_1 = a_2 = a_3 = \frac{1}{\sqrt{3}}$

Soln. Given the normalized wavefunction: $\phi = a_1 \psi_{11} + a_2 \psi_{10} + a_3 \psi_{1-1}$

Now, $\hat{L}_x \phi = \left[\frac{\hat{L}_+ + \hat{L}_-}{2}\right]\left[a_1 \psi_{11} + a_2 \psi_{10} + a_3 \psi_{1,-1}\right]$

Using the operations of the ladder operators i.e.

$$\hat{L}_+ \psi_{lm} = \sqrt{(l-m)(l+m+1)}\hbar \psi_{lm+1}$$
$$\hat{L}_- \psi_{lm} = \sqrt{(l+m)(l-m+1)}\hbar \psi_{lm-1}$$

So, $\hat{L}_x \phi = \frac{1}{2}\left[a_2.\sqrt{2}\hbar.\psi_{11} + a_3.\sqrt{2}\hbar.\psi_{10} + a_1.\sqrt{2}\hbar.\psi_{10} + a_2.\sqrt{2}\hbar.\psi_{1-1}\right]$

$$= \hbar\left[\frac{a_2}{\sqrt{2}}\psi_{11} + \frac{(a_3 + a_1)}{\sqrt{2}}\psi_{10} + \frac{a_2}{\sqrt{2}}\psi_{1-1}\right]$$

Since, ϕ is an eigenfunction of $\hat{L}_x$ with eigenvalue $\hbar$, therefore

$$a_1 = \frac{a_2}{\sqrt{2}}, a_3 = \frac{a_2}{\sqrt{2}} \text{ and } \frac{1}{\sqrt{2}}(a_3 + a_1) = a_2$$

So, $a_1 = a_3 = \frac{1}{2}$ and $a_2 = \frac{1}{\sqrt{2}}$

Correct answeris (b)

9. Let $\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$, where $\sigma_1, \sigma_2, \sigma_3$ are the Pauli matrices. If $\vec{a}$ and $\vec{b}$ are two arbitrary constant vectors in three dimensions, the commutator $[\vec{a}.\vec{\sigma}, \vec{b}.\vec{\sigma}]$ is equal to (in the following I is the identity matrix)

(a) $(\vec{a}\cdot\vec{b})(\sigma_1 + \sigma_2 + \sigma_3)$ (b) $2i(\vec{a}\times\vec{b})\cdot\vec{\sigma}$ **[CSIR Dec 2014]**

(c) $(\vec{a}\cdot\vec{b})I$ (d) $|\vec{a}||\vec{b}|I$

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Soln. Let assume, $\vec{a} = a_1\hat{i} + a_2\hat{j} + a_3\hat{k}$ and $\vec{b} = b_1\hat{i} + b_2\hat{j} + b_3\hat{k}$

Therefore,

$$\left[\vec{a}.\vec{\sigma}, \vec{b}.\vec{\sigma}\right] = \left[a_1\sigma_x + a_2\sigma_y + a_3\sigma_z, b_1\sigma_x + b_2\sigma_y + b_3\sigma_z\right]$$
$$= \left[a_1\sigma_x, b_1\sigma_x\right] + \left[a_1\sigma_x, b_2\sigma_y\right] + \left[a_1\sigma_x, b_3\sigma_z\right] + \left[a_2\sigma_y, b_1\sigma_x\right] + \ldots\ldots\ldots\ldots$$

Using the commutation relations, $\left[\sigma_x, \sigma_y\right] = 2i\sigma_z, \left[\sigma_y, \sigma_z\right] = 2i\sigma_x, \left[\sigma_z, \sigma_x\right] = 2i\sigma_y$, we get

$$\left[\vec{a}.\vec{\sigma}, \vec{b}.\vec{\sigma}\right] = 2i\left(a_1b_2\sigma_z - a_1b_3\sigma_y - a_2b_1\sigma_z + a_2b_3\sigma_x + a_3b_1\sigma_y - a_3b_2\sigma_x\right)$$
$$= 2i\left\{(a_2b_3 - a_3b_2)\sigma_x - (a_1b_3 - a_3b_1)\sigma_y + (a_1b_2 - a_1b_2)\sigma_z\right\} = 2i\left(\vec{a}\times\vec{b}\right).\vec{\sigma}$$

PRACTICE SET

1. Let $\vec{L}=(L_x,L_y,L_z)$ denote the orbital angular momentum operators of a particle and let $L_+ = L_x + iL_y$ and $L_- = L_x - iL_y$. The particle is in an eigenstate of L^2 and L_z eigenvalues $\ell(\ell+1)\hbar^2$ and $\hbar\ell$ respectively. The expectation value of $L_+ L_-$ in this state is: **[GATE 2001]**

(a) $\ell\hbar^2$ (b) $2\ell\hbar^2$ (c) 0 (d) $\ell\hbar$

2. An electron is in a state spin wave function $\phi_s = \begin{pmatrix} \sqrt{3}/2 \\ 1/2 \end{pmatrix}$ in the S_z representation. What is the probability of finding the z-componenet of its spin along the $-\hat{z}$ direction? **[GATE 2002]**

(a) 0.75 (b) 0.50 (c) 0.35 (d) 0.25

3. In a Stern-Gerlach experiment, the magnetic field is in +z direction. A particle comes out of this experiment in $|+\hat{z}\uparrow\rangle$ state. Which of the following statements is true? **[GATE 2002]**

(a) The particle has a definite value of the y-component of the spin angular momentum.
(b) The particle has a definite value of the square of the spin angular momentum.
(c) The particle has a definite value of x-components of spin angular momentum.
(d) The particle has definite values of x- and y-components of spin angular momentum.

4. A spin half particle is in the state $S_z = \hbar/2$. The expectation values of S_z, S_x^2, S_y, S_y^2 are given by **[GATE 2003]**

(a) $0,0,\hbar^2/4,\hbar^2/4$ (b) $0,\hbar^2/4,\hbar^2/4,0$ (c) $0,\hbar^2/4,0,\hbar^2/4$ (d) $\hbar^2/4,\hbar^2/4,0,0$

5. The commutator, $\left[L_z, Y_{\ell m}(\theta,\phi)\right]$ where L_z is the z component of the orbital angular momentum and $Y_{\ell m}(\theta,\phi)$ is a spherical harmonic, is: **[GATE 2005]**

(a) $\ell(\ell+1)\hbar$ (b) $-m\hbar$ (c) $m\hbar$ (d) $+\ell\hbar$

6. For a spin 1/2 particle, the expectation value of $s_x s_y s_z$, where s_x, s_y and s_z are spin operators, is **[GATE 2005]**

(a) $\frac{i\hbar^3}{8}$ (b) $\frac{i\hbar^3}{16}$ (c) $\frac{i\hbar^3}{8}$ (d) $-\frac{i\hbar^3}{16}$

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7. The commutator $[L_x, y]$, where L_x is the x-component of the angular momentum operator and y is the y-component of the position operator, is equal to: **[GATE 2006]**

(a) 0 (b) $i\hbar x$ (c) $i\hbar y$ (d) $i\hbar z$

8. Which one of the following relations is true for Pauli matrices? **[GATE 2006]**

(a) $\sigma_x\sigma_y = \sigma_y\sigma_x$ (b) $\sigma_x\sigma_y = \sigma_z$ (c) $\sigma_x\sigma_y = i\sigma_z$ (d) $\sigma_y\sigma_x = i\sigma_z$

9. Let $|\psi_0\rangle$ denote the ground state of the hydrogen atom. Choose the correct statement from those given below: **[GATE 2008]**

(a) $[L_x, L_y]|\psi_0\rangle = 0$ (b) $J^2|\psi_0\rangle = 0$ (c) $[\vec{L},\vec{S}]|\psi_0\rangle \neq 0$ (d) $[S_x, S_y]|\psi_0\rangle = 0$

10. $\sigma_i\,(i=1,2,3)$ represents the Pauli spin matrices. Which one of the following is NOT true? **[GATE 2009]**

(a) $\sigma_i\sigma_j+\sigma_j\sigma_i=2\delta_{ij}$ (b) $\mathrm{Tr}(\sigma_i)=0$

(c) The eigenvalues of σ_i are ±1 (d) $\det(\sigma_i)=1$

11. For a spin s particle, in the eigen basis of S^2, S_z the expectation value $\langle sm|S_x^2|sm\rangle$ is **[GATE 2010]**

(a) $\dfrac{\left[s(s+1)-m^2\right]\hbar^2}{2}$ (b) $\left[s(s+1)-2m^2\right]\hbar^2$ (c) $\left[s(s+1)-m^2\right]\hbar^2$ (d) $m^2\hbar^2$

12. If L_x, L_y and L_z are the x, y and z components of angular momentum operator L, the commutator $\left[L_xL_y, L_z\right]$ is equal to **[GATE 2011]**

(a) $i\hbar\left(L_x^2+L_y^2\right)$ (b) $i\hbar\left(L_x^2-L_y^2\right)$ (c) $2i\hbar L_z$ (d) zero

13. Which one of the following commutation relations is not correct? **[GATE 2013]**

(a) $\left[L^2, L_z\right]=0$ (b) $\left[L_x, L_y\right]=i\hbar L_z$ (c) $\left[L_z, L_+\right]=\hbar L_+$ (d) $\left[L_z, L_-\right]=\hbar L_-$

14. A spin-half particle is in a linear superposition $0.8|\uparrow\rangle+0.6|\downarrow\rangle$ of its spin-up and spin-down states. If $|\uparrow\rangle$ and $|\downarrow\rangle$ are the eigen states of σ_z, then what is the expectation value, up to one decimal place, of the operator $10\sigma_z+5\sigma_x$? ..... **[GATE 2013]**

15. If $\vec{L}$ is the orbital angular momentum and $\vec{S}$ is the spin angular momentum, then $\vec{L}.\vec{S}$ does not commute with **[GATE 2014]**

(a) S_z (b) L^2 (c) S^2 (d) $\left(\vec{L}+\vec{S}\right)^2$

16. ψ_1 and ψ_2 are two orthogonal states of a spin ½ system. it is given that

$$\psi_1=\frac{1}{\sqrt{3}}\begin{pmatrix}1\\0\end{pmatrix}+\sqrt{\frac{2}{3}}\begin{pmatrix}0\\1\end{pmatrix}$$ **[GATE 2014]**

where $\begin{pmatrix}1\\0\end{pmatrix}$ and $\begin{pmatrix}0\\1\end{pmatrix}$ represents the spin-up and spin-down states, respectively. When the system is in the state ψ_2, its probability to be in the spin-up state is _____

17. If L_+ and L_- are the angular momentum ladder operators, then the expectation value of $\left(L_+L_- + L_-L_+\right)$ in the state $|l=1, m=1\rangle$ of an atom is _____ $\hbar^2$. **[GATE 2014]**

18. Let $\vec{L}$ and $\vec{p}$ be the angular and linear momentum operators respectively, for a particle. The commutator $\left[L_x, p_y\right]$ gives **[GATE 2015]**

(a) $-i\hbar p_x$ (b) 0 (c) $i\hbar p_x$ (d) $i\hbar p_z$

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19. The Pauli spin matrices for three spin-1/2 particles are $\vec{\sigma}_1, \vec{\sigma}_2$ and $\vec{\sigma}_3$ respectively. The dimension of the Hilbert space required to define a operator $\hat{O} = \vec{\sigma}_1.(\vec{\sigma}_2 \times \vec{\sigma}_3)$ is _____

[GATE 2015]

20. An operator for a spin-1/2 particle is given by $\hat{A} = \lambda \vec{\sigma}.\vec{B}$, where $\vec{B} = \frac{B}{\sqrt{2}}(\hat{x} + \hat{y})$, $\vec{\sigma}$ denotes Pauli spin matrices and λ is a constant. The eigenvalue of $\hat{A}$ are **[GATE 2015]**

(a) $\pm\frac{\lambda B}{\sqrt{2}}$ (b) $\pm\lambda B$ (c) $0, \lambda B$ (d) $0, -\lambda B$

21. Consider the Hamiltonian

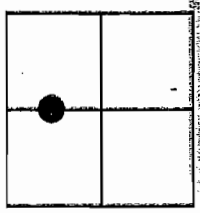
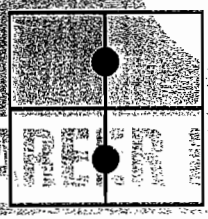
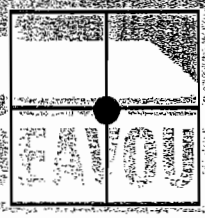
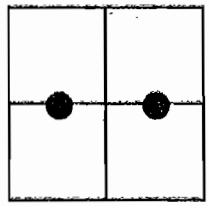
$$H = f\vec{\sigma}.\vec{x}$$

Here $\vec{x}$ is the position vector, f is a constant and $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$, where $\sigma_x, \sigma_y, \sigma_z$ are the three Pauli matrices. The energy eigenvalues are **[TIFR 2014]**

(a) $f\left(\sqrt{x^2 + y^2} \pm z\right)$ (b) $f(x \pm iy)$ (c) $\pm f\sqrt{x^2 + y^2 + z^2}$ (d) $\pm f(x + y + z)$

22. In a Stern-Gerlach experiment with spin-½ particles, the beam is found to form two spots on the screen, one directly above the other. The experimenter now makes a hole in the screen at the position of the upper spot. The particles that go through this hole are then passed through another Stern-Gerlach apparatus but with its magnets rotated by 90 degrees counter-clockwise about the axis of the beam direction. Which of the following shows what happens on the second screen?

[TIFR 2015]

(a)  (b)  (c)  (d) 

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23. An rigid rotator has the wave function **[TIFR 2015]**

$$\psi(\theta, \varphi) = N\left[2i\,Y_{1,0}(\theta, \varphi) + (2 + i)\,Y_{2,-1}(\theta, \varphi) + 3i\,Y_{1,1}(\theta, \varphi)\right]$$

where $Y_{l,m}(\theta, \varphi)$ are the sphereical harmonics, and N is a normalization constant. If $\vec{L}$ is the orbital angular momentum operator, and $L_\pm = L_x \pm iL_y$ the expectation value of L_+L_- is

(a) $\frac{21\hbar^2}{9}$ (b) $\frac{23\hbar^2}{9}$ (c) $\frac{25\hbar^2}{9}$ (d) 0

24. Define $\sigma_x = (f^\dagger + f)$ and $\sigma_y = -i(f^\dagger - f)$, where the σ^i are Pauli spin matrices and $f, f^\dagger$ obey anticommutation relations $\{f, f\} = 0, \{f, f^\dagger = 1\}$. Then σ_z is given by **[JEST 2012]**

(a) $f^\dagger f - 1$ (b) $2f^\dagger f - 1$ (c) $2f^\dagger f + 1$ (d) $f^\dagger f$

25. Consider a system of two spin-1/2 particles with total spin $\vec{S} = \vec{s}_1 + \vec{s}_2$, where s_1 and s_2 are in terms of Pauli matrices σ_i. The spin triplet projection operator is **[JEST 2012]**

(a) $\frac{1}{4} + s_1.s_2$ (b) $\frac{3}{4} - s_1.s_2$ (c) $\frac{3}{4} + s_1.s_2$ (d) $\frac{1}{4} - s_1.s_2$

26. Consider a spin-1/2 particle in the presence of homogeneous magnetic field of magnitude B along z-axis which is prepared initially in a state $|\psi\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle + |\downarrow\rangle\right)$ at time t = 0. At what time 't' will the particles be in the state $-|\psi\rangle$ (μ_B is Bohr magneton)? **[JEST 2012]**

(a) $t = \frac{\pi\hbar}{\mu_B B}$ (b) $t = \frac{2\pi\hbar}{\mu_B B}$ (c) $t = \frac{\pi\hbar}{2\mu_B B}$ (d) Never

27. If J_x, J_y, J_z are angular momentum operators, the eigenvalues of the operator $\left(J_x + J_y\right)/\hbar$ are **[JEST 2013]**

(a) real and discrete with rational spacing (b) real and discrete with irrational spacing
(c) real and continuous (d) not all real

28. Consider the state $\begin{pmatrix} 1/2 \\ 1/2 \\ 1/\sqrt{2} \end{pmatrix}$ corresponding to the angular momentum $l = 1$ in the L_z basis of states with m = +1,0,–1. If L_z^2 is measured in this state yielding a result 1, what is the state after the measurement? **[JEST 2013]**

(a) $\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$ (b) $\begin{pmatrix} 1/\sqrt{3} \\ 0 \\ \sqrt{2/3} \end{pmatrix}$ (c) $\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$ (d) $\begin{pmatrix} 1/\sqrt{2} \\ 0 \\ 1/\sqrt{2} \end{pmatrix}$

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29. What are the eigenvalues of the operator $\vec{\alpha}.\vec{\sigma}$, where $\vec{\sigma}$ are the three Pauli matrices and $\vec{\alpha}$ is a vector? **[JEST 2013]**

(a) $\alpha_x + \alpha_y$ and α_z (b) $\alpha_x + \alpha_y$ and $i\alpha_z$ (c) $\pm\left(\alpha_x + \alpha_y + \alpha_z\right)$ (d) $\pm|\vec{\alpha}|$

30. Consider an eigenstate of $\vec{L}^2$ and L_z operator denoted by $|\ell, m\rangle$. Let $A = \hat{n}.\vec{L}$ denote an operator, where $\hat{n}$ is a unit vector parametrized in terms of two angles as $\left(n_x, n_y, n_z\right) = \left(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta\right)$. The width ΔA in $|\ell, m\rangle$ state is: **[JEST 2014]**

(a) $\sqrt{\frac{\ell(+1) - m^2}{2}}\hbar\cos\theta$ (b) $\sqrt{\frac{\ell(+1) - m^2}{2}}\hbar\cos\theta$

(c) $\sqrt{\ell(\ell+1) - m^2}\hbar\sin\theta$ (d) $\sqrt{\ell(\ell+1) - m^2}\hbar\cos\theta$

31. Suppose a spin $\frac{1}{2}$ particle is in the state

$$|\psi\rangle = \frac{1}{\sqrt{6}}\begin{bmatrix} 1+i \\ 2 \end{bmatrix}$$

If S_x (x component of the spin angular momentum operator) is measured what is the probability of getting $+\frac{\hbar}{2}$? **[JEST 2014]**

(a) $\frac{1}{3}$ (b) $\frac{2}{3}$ (c) $\frac{5}{6}$ (d) $\frac{1}{6}$

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Chapter 5

Three-dimensional potentials

5.1 Three-Dimensional rectangular box :

We consider a free particle of mass m confined to move non-relativistically in a three-dimensional potential box of sides a, b and c parallel to the x, y and z-axes respectively. Since the particle is free, the potential inside the box is $V(x,y,z)=0$. So, the total energy of the particle inside the box is equal to its kinetic energy which is always a positive quantity.

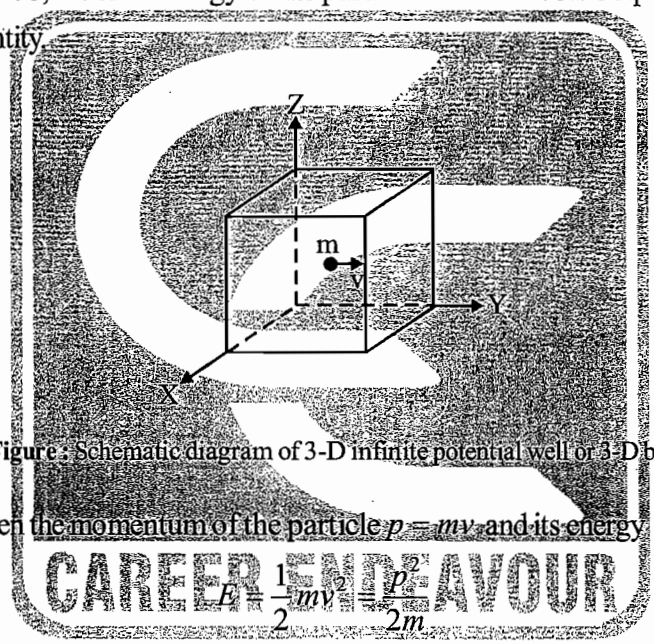

Figure : Schematic diagram of 3-D infinite potential well or 3-D box

If v be the velocity, then the momentum of the particle $p = mv$ and its energy

$$E = \frac{1}{2}mv^2 = \frac{p^2}{2m}$$

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Since the potential energy $V(x,y,z)$ is independent of time, we here apply Schrodinger time -independent 3-D wave equation to obtain the wave functiuon $\psi(x,y,z)$ and the eigenvalue of the energy of the particle.

The three-dimensional potential box has the following characteristics:

$$V(x,y,z)=\begin{cases}0, & \text{for } 0<x<a, 0<y<b, 0<z<c \\ \infty & \text{for } \quad x>a, \quad y>b, \quad z>c\end{cases} \tag{1}$$

The wave equation for the Particle:

The wave equation describing the motion of the particle can be written as

$$\hat{H}\psi = -\frac{\hbar^2}{2m}\nabla^2\psi = E\psi$$

$$\Rightarrow \frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}+\frac{2mE}{\hbar^2}\psi = 0 \tag{2}$$

As $V(x,y,z)=\infty$ at the boundries and outside the box $\psi(x,y,z)=0$ at the boundaries and outside potential box. The boundary conditions can be written as,

$$\left.\begin{aligned}\psi(x,y,z)=0 \text{ at } x=0 \text{ and } x=a\\ y=0 \text{ and } y=b\\ z=0 \text{ and } z=c\end{aligned}\right\}$$

Using the separation of variable technique, we caan assume the solution of equation (2) to be

$$\psi(x,y,z)=X(x)Y(y)Z(z) \tag{3}$$

Substituting equation (3) in equation (2), we get

$$YZ\frac{d^2X}{dx^2}+ZX\frac{d^2Y}{dy^2}+XY\frac{d^2Z}{dz^2}+\frac{2mE}{\hbar^2}XYZ=0$$

Dividing throughout by XYZ, we get

$$\frac{1}{X}\frac{d^2X}{dx^2}+\frac{1}{Y}\frac{d^2Y}{dy^2}+\frac{1}{Z}\frac{d^2Z}{dz^2}+\frac{2mE}{\hbar^2}=0 \tag{4}$$

If v_x, y_y and v_z be the component of velocity of the particle along the x, y and z-axes respectively, then the corresponding kinetic energies of the particle are

$$E_x=\frac{1}{2}mv_x^2,\quad E_y=\frac{1}{2}mv_y^2 \text{ and } E_z=\frac{1}{2}mv_z^2$$

such that $E=E_x+E_y+E_z$

Therefore, equation (4) can be written as

$$\left[\frac{1}{X}\frac{d^2X}{dx^2}+\frac{2mE_x}{\hbar^2}\right]+\left[\frac{1}{Y}\frac{d^2Y}{dy^2}+\frac{2mE_y}{\hbar^2}\right]+\left[\frac{1}{Z}\frac{d^2Z}{dz^2}+\frac{2mE_z}{\hbar^2}\right]=0 \tag{5}$$

So,

$$\frac{1}{X}\frac{d^2X}{dx^2}+\frac{2mE_x}{\hbar^2}X=0 \tag{6a}$$

$$\frac{1}{Y}\frac{d^2Y}{dy^2}+\frac{2mE_y}{\hbar^2}Y=0 \tag{6b}$$

$$\frac{1}{Z}\frac{d^2Z}{dz^2}+\frac{2mE_z}{\hbar^2}Z=0 \tag{6c}$$

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Solutions of equations (6a), (6b) and (6c) are

$$X(x)=A_1\sin k_x x+B_1\cos k_x x \text{ where } k_x=\frac{\sqrt{2mE_x}}{\hbar}$$

$$Y(y)=A_2\sin k_y y+B_2\cos k_y y \text{ where } k_y=\frac{\sqrt{2mE_y}}{\hbar}$$

$$Z(z)=A_3\sin k_z z+B_3\cos k_z z \text{ where } k_z=\frac{\sqrt{2mE_z}}{\hbar}$$

Boundary Conditions:

(i) $X(x=0)=0 \Rightarrow B_1=0$

$$X(x=a)=0 \Rightarrow A\sin k_x a=0 \quad \Rightarrow \sin k_x a=0 \quad \Rightarrow k_x=\frac{n_x\pi}{a} \quad (n_x=1,2,3.....)$$

(ii) $Y(y=0)=0 \Rightarrow B_2=0$

$$Y(y=b)=0 \Rightarrow A_2\sin k_y a=0 \quad \Rightarrow \sin k_y a=0 \quad \Rightarrow k_y=\frac{n_y\pi}{a} \quad (n_y=1,2,3.....)$$

(iii) $Z(z=0)=0 \Rightarrow B_3=0$

$$Z(z=c)=0 \Rightarrow A_3\sin k_z a=0 \quad \Rightarrow \sin k_z a=0 \quad \Rightarrow k_z=\frac{n_z\pi}{a} \quad (n_z=1,2,3.....)$$

Therefore, the solution will become

$$\psi(x,y,z)=A_1A_2A_3\sin\frac{n_x\pi}{a}x\sin\frac{n_y\pi}{b}y\sin\frac{n_z\pi}{c}z$$

$$\Rightarrow\psi(x,y,z)=A\sin\frac{n_x\pi}{a}x\sin\frac{n_y\pi}{b}y\sin\frac{n_z\pi}{c}z \qquad (7)$$

Normalization Condition:

$$\int_0^a\int_0^b\int_0^c|\psi|^2dxdydz=1$$

$$\Rightarrow A^2\int_0^a\int_0^b\int_0^c\sin^2\frac{n_x\pi}{a}x\sin^2\frac{n_y\pi}{b}y\sin^2\frac{n_z\pi}{c}zdxdydz=1$$

$$\Rightarrow A^2.\frac{a}{2}.\frac{b}{2}.\frac{c}{2}=1\Rightarrow A=\sqrt{\frac{8}{abc}}$$

Now, the eigenfunction of the particle is,

$$\psi(x,y,z)=\sqrt{\frac{8}{abc}}\sin\frac{n_x\pi}{a}x\sin\frac{n_y\pi}{b}y\sin\frac{n_z\pi}{c}z \qquad (8)$$

Therefore, the total linear momentum p is $p=p_x^2+p_y^2+p_z^2$

$$=\left[\left(\frac{n_x\hbar\pi}{a}\right)^2+\left(\frac{n_y\hbar\pi}{b}\right)^2+\left(\frac{n_z\hbar\pi}{c}\right)^2\right]^{1/2}=\pi\hbar\left[\left(\frac{n_x}{a}\right)^2+\left(\frac{n_y}{b}\right)^2+\left(\frac{n_z}{c}\right)^2\right]$$

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The eigenvalue of energy of the particle is,

$$E=\frac{p^2}{2m}=\frac{\pi^2\hbar^2}{2m}\left[\left(\frac{n_x}{a}\right)^2+\left(\frac{n_y}{b}\right)^2+\left(\frac{n_z}{c}\right)^2\right]$$

The integers n_x, n_y, n_z are called quantum numbers which are required to describe the stationary state of the particle. Since for any of n_x, n_y, n_z being zero, $\psi(x,y,z)=0$, i.e., the particle is absent in the box. But physically this is not acceptable and hence any of n_x, n_y, n_z cannot be zero.

For the ground state, $n_x=n_y=n_z=1$ and the ground state wave function of the particle is,

$$\psi_{1,1,1}(x,y,z)=\sqrt{\frac{8}{abc}}\sin\frac{\pi x}{a}\sin\frac{\pi y}{b}\sin\frac{\pi z}{c}$$

and the energy associated with the ground state called the zero point energy is given by,

$$E_{1,1,1} = \frac{\pi^2\hbar^2}{2m}\left[\frac{1}{a^2}+\frac{1}{b^2}+\frac{1}{c^2}\right]$$

The eigenfunctions and eigenvalues of energy for the next higher excited state are as follows:

$$\left.\begin{aligned}\psi_{2,1,1} &= \sqrt{\frac{8}{abc}}\sin\frac{2\pi x}{a}\sin\frac{\pi y}{b}\sin\frac{\pi z}{c}\\ \psi_{1,2,1} &= \sqrt{\frac{8}{abc}}\sin\frac{\pi x}{a}\sin\frac{2\pi y}{b}\sin\frac{\pi z}{c}\\ \psi_{1,1,2} &= \sqrt{\frac{8}{abc}}\sin\frac{\pi x}{a}\sin\frac{\pi y}{b}\sin\frac{2\pi z}{c}\end{aligned}\right\} \text{ and } \left.\begin{aligned}E_{2,1,1} &= \frac{\pi^2\hbar^2}{2m}\left[\frac{4}{a^2}+\frac{1}{b^2}+\frac{1}{c^2}\right]\\ E_{1,2,1} &= \frac{\pi^2\hbar^2}{2m}\left[\frac{1}{a^2}+\frac{4}{b^2}+\frac{1}{c^2}\right]\\ E_{1,1,2} &= \frac{\pi^2\hbar^2}{2m}\left[\frac{1}{a^2}+\frac{1}{b^2}+\frac{4}{c^2}\right]\end{aligned}\right\}$$

5.2 Three-dimensional cubical box:

If the potential box be cubical instead of rectagular, then $a = b = c$ the eigenfunction corresponding to the state of the particle will be represented by

(7)

$$\psi_{n_x n_y n_z}(x,y,z) = \sqrt{\frac{8}{a^3}}\sin\frac{n_x\pi}{a}x\sin\frac{n_y\pi}{a}y\sin\frac{n_z\pi}{a}z$$

The momentum eigenvalues of the particle will be,

$$p_{n_x n_y n_z} = \frac{\pi\hbar}{a}\left[n_x^2+n_y^2+n_z^2\right]^{\frac{1}{2}}$$

and the corresponding energy eigenvalues are, $E_{n_x n_y n_z} = \frac{\pi^2\hbar^2}{2ma^2}\left[n_x^2+n_y^2+n_z^2\right]$

Ground state ($n_x = n_y = n_z = 1$):

(8)

Wave function: $\psi_{1,1,1} = \sqrt{\frac{8}{a^3}}\sin\frac{\pi x}{a}\sin\frac{\pi y}{a}\sin\frac{\pi z}{a}$

Momentum : $p_{1,1,1} = \frac{\pi\hbar}{a}\sqrt{3}$ **Energy :** $E_{1,1,1} = \frac{3\pi^2\hbar^2}{2ma^2}$

First excited state:

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n_x	n_y	n_z
2	1	1
1	2	1
1	1	2

Wave function: $\left.\begin{aligned}\psi_{2,1,1} &= \sqrt{\frac{8}{a^3}}\sin\frac{2\pi x}{a}\sin\frac{\pi y}{a}\sin\frac{\pi z}{a}\\ \psi_{1,2,1} &= \sqrt{\frac{8}{a^3}}\sin\frac{\pi x}{a}\sin\frac{2\pi y}{a}\sin\frac{\pi z}{a}\\ \psi_{1,1,2} &= \sqrt{\frac{8}{a^3}}\sin\frac{\pi x}{a}\sin\frac{\pi y}{a}\sin\frac{2\pi z}{a}\end{aligned}\right\}$

of the

. But

Momentum: $p_{2,1,1} = p_{1,2,1} = p_{1,1,2} = \frac{\pi\hbar}{a}\sqrt{6}$

Energy: $E_{2,1,1} = E_{1,2,1} = E_{1,1,2} = \frac{\pi^2\hbar^2}{2ma^2}6$

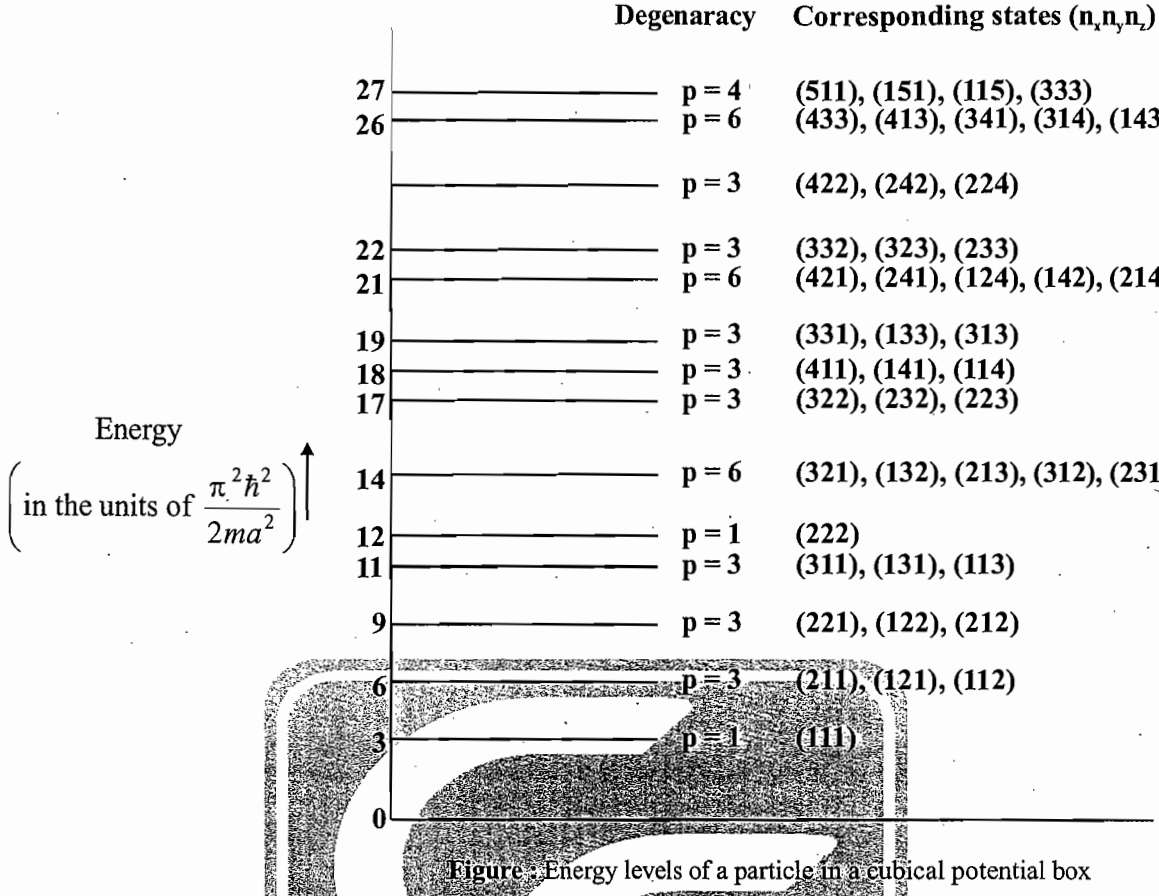

Figure : Energy levels of a particle in a cubical potential box

Degeneracy:

The property that, two or more quantum states of a particle, with different sets of quantum numbers and different eigenfunctions having the same value of momentum and energy is called degeneracy.

For example, the three states corresponding to quantum numbers (2, 1, 1), (1, 2, 1) and (1, 1, 2) all have the same momentum $\left(\frac{\pi\hbar}{a}\sqrt{6}\right)$ and energy $\left(\frac{\pi^2\hbar^2}{2ma^2}6\right)$.

Example 1. An electron is confined in a cubical box of side 1 Å. Find the momentum and energy of the electron in the ground state and the first excited state.

Soln. Ground state: $n_x = n_y = n_z = 1$

Momentum of the electron is

$$P_{1,1,1} = \frac{\pi\hbar}{\ell}\sqrt{3} = \frac{\pi h}{2\pi\ell}\sqrt{3} = \frac{h}{2\ell}\sqrt{3} = 5.72\times10^{-24}\,kg-m/s$$

Energy of the electron is

$$E_{1,1,1} = \frac{3\pi^2\hbar^2}{2m\ell^2} = 181\times10^{-19}\,J = 113\,eV$$

First excited state:

n_x	n_y	n_z
2	1	1
1	2	1
1	1	2

Momentum of the electron: $p_{2.1.1} = p_{1.2.1} = p_{1,1,2} = \frac{\pi\hbar}{a}\sqrt{6} = 8.13\times10^{-24}\,kg-m/s$

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Energy of the electron : $E_{2,1,1} = E_{1,2,1} = E_{1,1,2} = \dfrac{\pi^2\hbar^2}{2ma^2}6 = 362\times10^{-19}\,J = 226\,eV$

Example 2. An electron is confined in a cubical box of side 1Å. (i) Find its lowest energy (ii) what is the temperature at which the average of the molecule of a perfect gas would be equal to the lowest energy of the electron $\left(k = 1.38\times10^{-23}\ J/K\right)$?

Soln. (i) Ground state energy of the electron

$$E_{1,1,1} = \frac{3\pi^2\hbar^2}{2ma^2} = \frac{3\pi^2\times\left(1.054\times10^{-34}\right)^2}{2\times9.11\times10^{-31}\times\left(10^{-10}\right)^2} = 18.03\times10^{-18}\,J$$

(ii) If T K be the required temeprature of the molecules, then

$$\frac{3}{2}kT = \frac{3\pi^2\hbar^2}{2ma^2}$$ [k is the Boltzmann constant]

$$= 18.03\times10^{-18}\,J$$

$$\therefore \quad T = \frac{2\times18.03\times10^{-18}}{3\times1.38\times10^{-23}} = 8.71\times10^5\,K$$

Example 3. A particle of mass 'm' is in a cubic box of size 'a'. If the particle is in an eigenstate with energy $E = \dfrac{14\pi^2\hbar^2}{2ma^2}$. What will be its wave function?

Soln. $E = \dfrac{14\pi^2\hbar^2}{2ma^2} = \dfrac{\pi^2\hbar^2}{2ma^2}\left(n_x^2+n_y^2+n_z^2\right) \quad \Rightarrow n_x^2+n_y^2+n_z^2 = 14$

$$\left(n_x, n_y, n_z\right) = (1,2,3)$$

$$\psi_{123}(x,y,z) = \sqrt{\frac{8}{a^3}}\sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{2\pi y}{a}\right)\sin\left(\frac{3\pi z}{a}\right)$$

$$= \left(\frac{2}{a}\right)^{3/2}\sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{2\pi y}{a}\right)\sin\left(\frac{3\pi z}{a}\right)$$

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Example 4. Find the number of energy states and energy levels in the range $E < [15\hbar^2/(8ma^2)]$ of a cubical box of side a.

Soln. For a particle in a cubic box of side a, the energy is given by

$$E = \frac{\pi^2h^2}{2ma^2}(n_x^2+n_y^2+n_z^2) = \frac{h^2}{8ma^2}(n_x^2+n_y^2+n_z^2)$$

Comparing with the given expression, we get $n_x^2+n_y^2+n_z^2 < 15$

The number of possible combinations of $(n_x\ n_y\ n_z)$ is

(1 1 1)	1 way
(1 1 2), (1 2 1), (2 1 1)	3 ways
(1 1 3), (1 3 1), (3 1 1)	3 ways
(1 2 2), (2 1 2), (2 2 1)	3 ways
(2 2 2)	1 way

(1 2 3), (1 3 2), (2.1 3), (3 2 1), (3 1 2)	6 ways
Total	17 ways

Hence the No. of possible states = 17. The No. of energy levels = 6.

Example 5. A crystal has some negative ion vacancies, each containing one electron. Treat these electrons as moving freely inside a volume whose dimensions are of the order of lattice constant. Assuming the value of lattice constant, estimate the longest wavelength of electromagnetic radiation absorbed by these electrons.

Soln. The energy levels of an electron in a cubical box of side a is

$$E_{n_x,n_y,n_z} = \frac{\pi^2\hbar^2}{2ma^2}(n_x^2+n_y^2+n_z^2), \quad n_x,n_y,n_z = 1,2,3,...$$

Lattice constant a = 1 Å = 10^{-10} m.

The energy of the ground state is given by

$$E_{1111} = \frac{\pi^2\hbar^2}{2ma^2}\times 3 = 1.795\times 10^{-17} J$$

The longest wavelength corresponds to the transition from energy E_{111} to E_{211}, and hence

$$E_{211} = \frac{\pi^2\hbar^2\times 6}{2ma^2} = 3.59\times 10^{-17}\ \text{J}$$

Longest wavelength $\lambda = \frac{c}{\nu} = \frac{ch}{E_{211}-E_{111}} = 11\ nm$

5.3 Three-dimensional harmonic oscillator :

We consider a particle of mass m bound to the origin by a force having components.

$$F_x = -k_x x = -m\omega_x^2 x$$

$$F_y = -k_y x = -m\omega_y^2 y$$

$$F_z = -k_z z = -m\omega_z^2 z$$

along the x, y, z components of the displacement r from the origin. Here k_x, k_y, k_z are the force constants and $\omega_x, \omega_y, \omega_z$ are the angular frequencies along x, y, z-axes respectively. Such a system is called a three-dimensional harmonic oscillator.

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Again, $F_x = -\frac{\partial V}{\partial x}$, $F_y = -\frac{\partial V}{\partial y}$ and $F_z = -\frac{\partial V}{\partial z}$

where the potential energy V of the oscillator is,

$$V(x,y,z) = \frac{1}{2}\left(k_x x^2 + k_y y^2 + k_z z^2\right)$$

The time-independent three-dimensional Schrodinger equation for the system is

$$-\frac{\hbar^2}{2m}\nabla^2\psi(x,y,z) + \frac{1}{2}\left(k_x x^2 + k_y y^2 + k_z z^2\right)\psi(x,y,z) = E\psi(x,y,z)$$

$$\Rightarrow \frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}+\frac{2m}{\hbar^2}\left[E-\frac{1}{2}k_x x^2-\frac{1}{2}k_y y^2-\frac{1}{2}k_z z^2\right]=0$$

$$\Rightarrow \frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}+\left[\lambda-\left(\alpha_x^2x^2+\alpha_y^2y^2+a_z^2z^2\right)\right]\psi=0 \qquad (9)$$

where, $\lambda=\frac{2mE}{\hbar^2}, \alpha_x=\sqrt{\frac{mk_x}{\hbar^2}}, \alpha_y=\sqrt{\frac{mk_y}{\hbar^2}}$ and $\alpha_z=\sqrt{\frac{mk_y}{\hbar^2}}$

Equation (9) can be solved by the method of separation of variables. The energy eigenvalues and eigenfunctions of the three-dimensional oscillator are therefore,

$$\left.\begin{aligned}E_x&=\left(n_x+\frac{1}{2}\right)\hbar\omega_x\\ E_y&=\left(n_y+\frac{1}{2}\right)\hbar\omega_y\\ E_z&=\left(n_z+\frac{1}{2}\right)\hbar\omega_z\end{aligned}\right\}$$

where, n_x, n_y and n_z are positive integers i.e., $n_x, n_y, n_z = 1, 2, 3, \ldots\ldots$ and

$X(x)=N_{n_x}\,e^{-\alpha_x^2x^2/2}H_{n_x}(\alpha_x x);\ Y(y)=N_{n_y}\,e^{-\alpha_y^2y^2/2}H_{n_y}(\alpha_y y);\ Z(z)=N_{n_z}\,e^{-\alpha_z^2z^2/2}H_{n_z}(\alpha_z z)$

Therefore, the complete wave function is

$$\psi_{n_xn_yn_z}=N_{n_x}N_{n_y}N_{n_z}\,e^{-\left(\alpha_x^2x^2+\alpha_y^2y^2+a_z^2z^2\right)/2}H_{n_x}(\alpha_x x)H_{n_y}(\alpha_y y)H_{n_y}(\alpha_z z) \qquad (10)$$

where the normalization factor is

$$N_{n_xn_yn_z}=\left[\frac{\alpha_x\alpha_y\alpha_z}{\pi^{3/2}2^{(n_x+n_y+n_z)}n_x!n_y!n_z!}\right]^{1/2}$$

$$E_{n_xn_yn_z}=\hbar\left[\left(n_x+\frac{1}{2}\right)\omega_x+\left(n_y+\frac{1}{2}\right)\omega_y+\left(n_z+\frac{1}{2}\right)\omega_z\right]$$

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For the isotropic oscillator, $\omega_x=\omega_y=\omega_z$ and $\alpha_x=\alpha_y=\alpha_z$

$$\therefore \quad E_n=\left[n_x+n_y+n_z+\frac{3}{2}\right]\hbar\omega=\left(n+\frac{3}{2}\right)\hbar\omega$$

where $n=n_x+n_y+n_z$ is the total quantum number and n = 0, 1, 2, 3, ...

It can be shown that except for the lowest energy level $\left(n_x=n_y=n_z=0, i.e.\ n=0\right)$ all the energy levels are degenerate.

The zero point (or, the ground level) energy E_0 for $n_x=n_y=n_z=0$ of the oscillator is given by

$$E_0=\frac{3}{2}\hbar\omega$$

Thus the zero point energy of a three-dimensional isotropic harmonic oscillator is three times that for the linear harmonic oscillator. the ground level of the oscillator is thus non-degenerate.

The state with principal quantum number n = 1, there are three levels each of energy $\frac{5}{2}\hbar\omega$. So, the first excited state is 3-fold degenerate. Similary, the state with n = 2 is 6-fold degenerate. Thus all the energy levels of the isotropic three-dimensional oscillator are degenerate and the degree of degeneracy is $p=\frac{1}{2}(n+1)(n+2)$.

Figure shows some of the energy levels of the oscillator.

n_x	n_y	n_z	n	Wave function	E_n	Degeneracy (p)
0	0	0	0	$\psi_{0,0,0}$	$\frac{3}{2}\hbar\omega$	$p=1$
1	0	0	1	$\psi_{1,0,0}$	$\frac{3}{2}\hbar\omega$	$p=3$
0	1	0		$\psi_{0,1,0}$		
0	0	1		$\psi_{0,0,1}$		
1	1	0	2	$\psi_{1,1,0}$	$\frac{3}{2}\hbar\omega$	$p=6$
1	0	1		$\psi_{1,0,0}$		
0	1	1		$\psi_{0,1,1}$		
2	0	0		$\psi_{2,0,0}$		
0	2	0		$\psi_{0,2,0}$		
0	0	2		$\psi_{0,0,2}$		

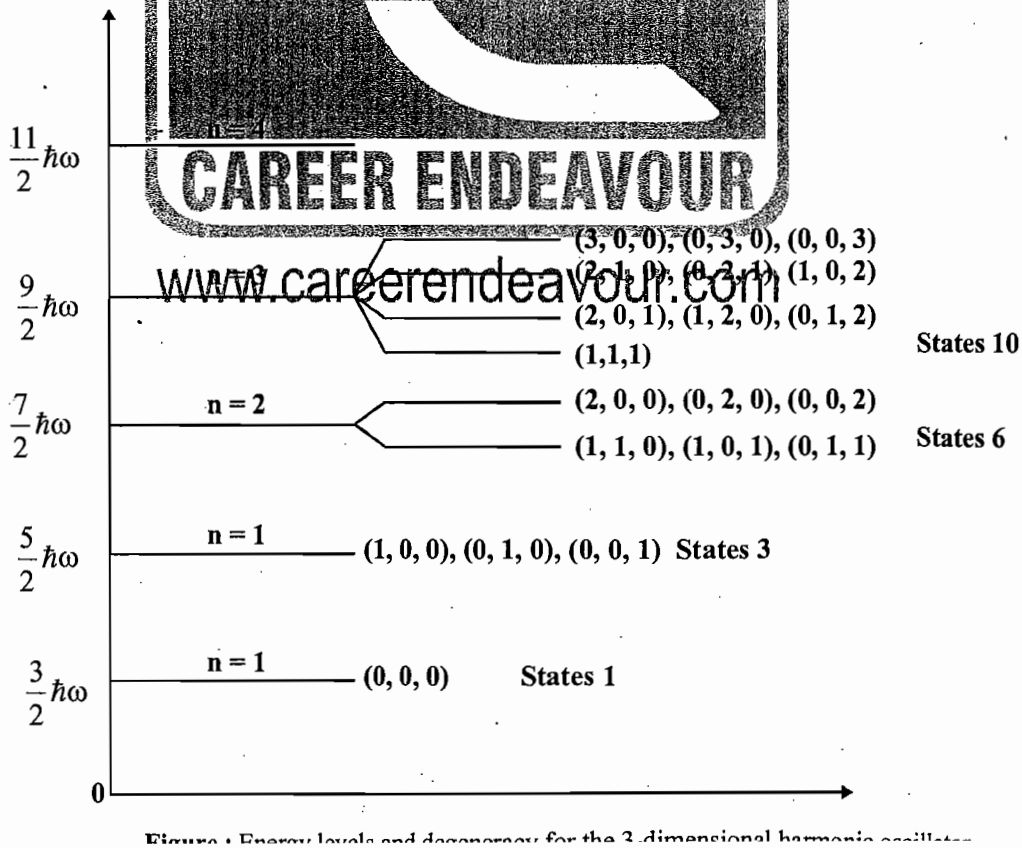
n = 4
n = 3
n = 2
n = 1
n = 1
$\frac{11}{2}\hbar\omega$
$\frac{9}{2}\hbar\omega$
$\frac{7}{2}\hbar\omega$
$\frac{5}{2}\hbar\omega$
$\frac{3}{2}\hbar\omega$
0
(3, 0, 0), (0, 3, 0), (0, 0, 3)
(2, 1, 0), (0, 2, 1), (1, 0, 2)
(2, 0, 1), (1, 2, 0), (0, 1, 2)
(1,1,1)
States 10
(2, 0, 0), (0, 2, 0), (0, 0, 2)
(1, 1, 0), (1, 0, 1), (0, 1, 1)
States 6
(1, 0, 0), (0, 1, 0), (0, 0, 1) States 3
(0, 0, 0) States 1

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Figure : Energy levels and degeneracy for the 3-dimensional harmonic oscillator

5.4 Spherically symmetric potentials :

We consider a particle of mass m moving in three dimensions under the influence of a force exerted by another particle located at the origin. The force is represented by $\vec{F} = -\nabla V(\vec{r})$, where, $\vec{r}$ is the distance of the particle from the origin.

If $V(r)$ depends only on r and not on the direction of r. Such a potential, which depend only r and not on θ and ϕ, is called a spherically symmetric potential.

The time-independent Schrodinger equation, for a particle moving in a spherical symmetric potential, in polar coordinates is given by

$$\nabla^2(r,\theta,\phi)+\frac{2m}{\hbar^2}\left[E-V(r)\right]\psi(r,\theta,\phi)=0 \tag{11}$$

Now, ∇^2 in spherical polar coordinates is given by,

$$\nabla^2=\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}$$

From equation (11) we get,

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}+\frac{2m}{\hbar^2}\left[E-V(r)\right]\psi=0 \tag{12}$$

But, $V(r)$ is a function of r and does not depend on θ and ϕ. So we can use the method of separation of variable. We therefore, write

$$\psi(r,\theta,\phi)=R(r)\Omega(\theta,\phi) \tag{13}$$

where, $R(r)$ and $\Omega(\theta,\phi)$ are the radial part and angular part of $\psi(r,\theta,\psi)$ respectively.

Using equation (13) in equation (12) and then dividing by $R(r)\Omega(\theta,\phi)$

We get,

$$\frac{1}{R(r)}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{1}{\Omega(\theta,\phi)\sin\theta}\left[\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Omega(\theta,\phi)}{\partial\theta}\right)\right]$$

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$$\frac{1}{\Omega(\theta,\phi)}\frac{1}{\sin^2\theta}\frac{\partial^2\Omega(\theta,\phi)}{\partial\phi^2}+\frac{2mr^2}{\hbar^2}\left[E-V(r)\right]=0 \tag{14}$$

In equation (14), the second and third terms are independent of r whereas the first and fourth terms dependent on r. So, we can write,

$$\frac{1}{\Omega(\theta,\phi)}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Omega(\theta,\phi)}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2\Omega(\theta,\phi)}{\partial\phi^2}\right]=C \tag{15}$$

and

$$-\frac{1}{R(r)}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)-\frac{2mr^2}{\hbar^2}\left[E-V(r)\right]=C \tag{16}$$

where, C is a constant.

Solution of the Angular part:

Equation (15) is independent of $V(r)$, so the solution giving the angular part of the wave function $\psi(r,\theta,\phi)$ will be the same for all spherical potentials. Further, equation (15) is related to angular momentum in the following way:

$$L^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]$$

So,
$$L^2\Omega(\theta,\phi) = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Omega(\theta,\phi)}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2\Omega(\theta)}{\partial\phi^2}\right]$$

$$= -\hbar^2 C\Omega(\theta,\phi)$$

Therefore,
$$L^2\Omega(\theta,\phi) = \lambda\Omega(\theta,\phi) \qquad (17)$$

Clearly, equation (17) is the eigenvalue equation for the operator $L^2\cdot\Omega(\theta,\phi)$ and λ are the eigenfunction and eigenvalue respectively belonging to the operator L^2.

Thus the normalised function $\Omega(\theta,\phi)$ are given by spherical harmonics i.e.

$$Y_\ell^m(\theta,\phi) = \left[\frac{(2\ell+1)(\ell-m)!}{4\pi(\ell+m)!}\right]^{1/2}(-1)^m e^{im\phi}P_\ell^m(\cos\theta), \text{ where } 0\le m\le\ell.$$

Some of spherical harmonics for $\ell=0,1$ and 2 are listed below:-

For $\ell=0$:
$$Y_0^0(\theta,) = \left(\frac{1}{4\pi}\right)^{1/2}$$

For $\ell=1$:
$$Y_1^1(\theta,\phi) = -\left(\frac{3}{8\pi}\right)^{1/2}\sin\theta\, e^{i\phi}$$

$$Y_1^0(\theta,\phi) = \left(\frac{3}{4\pi}\right)^{1/2}\cos\theta$$

$$Y_1^{-1}(\theta,\phi) = \left(\frac{3}{8\pi}\right)^{1/2}\sin\theta e^{-i\phi}$$

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For $\ell=2$:

$$Y_2^2(\theta,) = \frac{1}{4}\left(\frac{15}{2\pi}\right)^{1/2}\sin^2\theta\, e^{2i\phi}$$

$$Y_2^1(\theta,\phi) = -\left(\frac{15}{8\pi}\right)^{1/2}\sin\theta\cos\theta e^{-i\phi}$$

$$Y_2^0(\theta,) = \left(\frac{5}{4\pi}\right)^{1/2}\frac{3\cos^2\theta-1}{2}$$

$$Y_2^{-1}(\theta,\phi) = \left(\frac{15}{8\pi}\right)^{1/2}\sin\theta\cos\theta\, e^{-i\phi}$$

$$Y_2^{-2}(\theta,\phi) = \frac{1}{4}\left(\frac{15}{2\pi}\right)^{1/2}\sin^2\theta\, e^{-2i\phi}$$

Normalization condition of the function $Y_\ell^{m\ell}(\theta,\phi)$:

$$\int_{\theta=0}^{\pi}\int_{\Phi=0}^{2\pi} Y^*_{l,m_l}(\theta,\phi)\,Y_{l,m_l}(\theta,\phi)\sin\theta\,d\theta\,d\phi = 1$$

Solution of $R(r)$ equation: The radial part of the Schrodinger equation is,

$$-\frac{1}{R(r)}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)-\frac{2m}{\hbar^2}r^2\left[E-V(r)\right]=C=-\ell(\ell+1)\qquad\left[\because C=-\ell(\ell+1)\right]$$

$$\Rightarrow\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\left\{\frac{2m}{\hbar^2}\left[E-V(r)\right]-\frac{\ell(\ell+1)}{r^2}\right\}R=0 \qquad (18)$$

Now, $\psi(r,\theta,\phi)=R(r)\Theta(\theta)\Phi(\phi)=R(r)\Omega(\theta,\phi)=R(r)Y_\ell^{m\ell}(\theta,\phi)$

This is the complete three-dimensional wave function of the Schrodinger wave equation for a particle moving in a spherically symmetric $V(r)$. For a bound system, the wave function must satisfy the condition that

$$R(r)\to 0,\ \text{as}\ r\to\infty$$

If $V(r)$ is known, then only an explicit solution of (18) can be found out. Since equation (18) depend on n and l can have a discrete set of values, the allowed energy values must be discrete say, $E_1^\ell, E_2^\ell, \ldots\ldots, E_n^\ell$. The complete wave function of the particle corresponding to energy E_n^ℓ can be written as

$$\psi_{n,\ell,m_l}=R_n^\ell(r)\,Y_{l,m_l}(\theta,\phi)$$

As m_ℓ has $(2\ell+1)$ values, ranging from $-\ell$ to $+\ell$ in integral steps, there will be $(2\ell+1)$ wave function, each differing in m_ℓ values. Thus the energy state of the particle is $(2\ell+1)$ fold degenerate. The quantities n,ℓ and m_ℓ are known as the principal quantum number, orbital quantum number and azimuthal quantum number respectively. These quantum numbers are needed to specify the different states.

5.5 Hydrogen atom :

The simplest of the atoms is the hydrogen atom, consisting of a single electron moving around the nucleus containing only one nucleon (the proton) under a central force arising out of the Coulombian electrostatic attractive force. It forms the basis for the theoretical formulation of more complex atomic systems containing more than one electron. The old quantum theory was first proposed by N. Bohr (in 1912) on the basis of hydrogen atom. Schrodinger gave the solution of the wave equation for hydrogen atom is 1926 formulating the wave mechanics. There was extensive development of quantum theory of the hydrogen atom by the subsequent workers, viz, W. Heisenberg, max Born and Jordon and Pauli.

The results of hydrogen atom was successfully extended to other hydrogenic atoms. The hydrogenic atoms are of two types:

(i) Ionised atoms containing only one electron moving around the nucleus, which may consist of more than one proton and neutron. Singly ionised Helium (He^+), doubly ionised Lithium (Li^{++}), triply ionised Beryllium (Be^{+++}) are some of the hydrogenic atoms.

(ii) Atoms or, ions with closed shells and only one electron in the outermost shell form the second type of hydrogenic atoms. Atoms of alkali metal and alkaline earth ions are the examples.

The wave equation for the hydrogen atom:

The hydrogen or, hydrogenic atom is a two-particle system consisting of an electron of charge $-e$ moving round the nucleus of charge $+Ze$. The electron in this system moves under the central force arising out of the Coulombic electrostatic attraction between the nucleus and the electron along the radius of the circular path of motion.

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The potential energy of the system in absence of any external field is,

$$V(r) = \frac{1}{4\pi\varepsilon_0}\frac{ze^2}{r}$$

The potential energy is indepenent of θ and ϕ and thus spherically symmetric. Reducing the two body problem into one body problem, the 3-D Schrodinger equation in spherical polar coordinates can be written as

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\right)\frac{\partial\psi}{\partial r} + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2} + \frac{2\mu}{\hbar^2}\left[E - V(r)\right]\psi = 0$$

where $\mu = \dfrac{m_{nucleus}m_e}{m_{nucleus}+m_e}$ is the reduced mass of the system.

Using separation of variable technique, one can find the soluion of the above equation to be

$$\psi(r,\theta,\phi) = R_{nl}(r)\Theta_{lm}(\theta)\Phi_m(\phi)$$

where

$$R_{nl}(r) = \left[\left(\frac{2z}{na_0}\right)^3\frac{(n-l-1)!}{2n\left[(n+l)!\right]^3}\right]^{1/2} e^{-\frac{zr}{na_0}}\left(\frac{2zr}{na_0}\right)^l L_{n+l}^{2l+1}\left(\frac{2zr}{na_0}\right)$$

$$\Theta_{lm}(\theta) = \left[\sqrt{\frac{(2l+1)(l-m)!}{2.(l+m)!}}\right] P_l^m(\cos\theta)$$

$$\Phi(\phi) = \frac{1}{\sqrt{2\pi}}e^{im\phi}$$

Table : Normalised radial wave functions:

n	ℓ	$R_{nl}(r)$
1	0	$2\left(\frac{1}{a_0}\right)^{3/2} e^{-r/a_0}$
2	0	$\frac{1}{2\sqrt{2}}\left(\frac{1}{a_0}\right)^{3/2}\left(2-\frac{r}{a_0}\right)e^{-r/2a_0}$
2	1	$\frac{1}{2\sqrt{6}}\left(\frac{1}{a_0}\right)^{3/2}\frac{r}{a_0}e^{-r/2a_0}$
3	0	$\frac{2}{81\sqrt{3}}\left(\frac{1}{a_0}\right)^{3/2}\left(27-18\frac{r}{a_0}+2\frac{r^2}{a_0^2}\right)e^{-r/3a_0}$
3	1	$\frac{4}{81\sqrt{6}}\left(\frac{1}{a_0}\right)^{3/2}\left(6-\frac{r}{a_0}\right)\frac{r}{a_0}e^{-r/3a_0}$
3	2	$\frac{4}{81\sqrt{30}}\left(\frac{1}{a_0}\right)^{3/2}\frac{r^2}{a_0^2}e^{-r/3a_0}$

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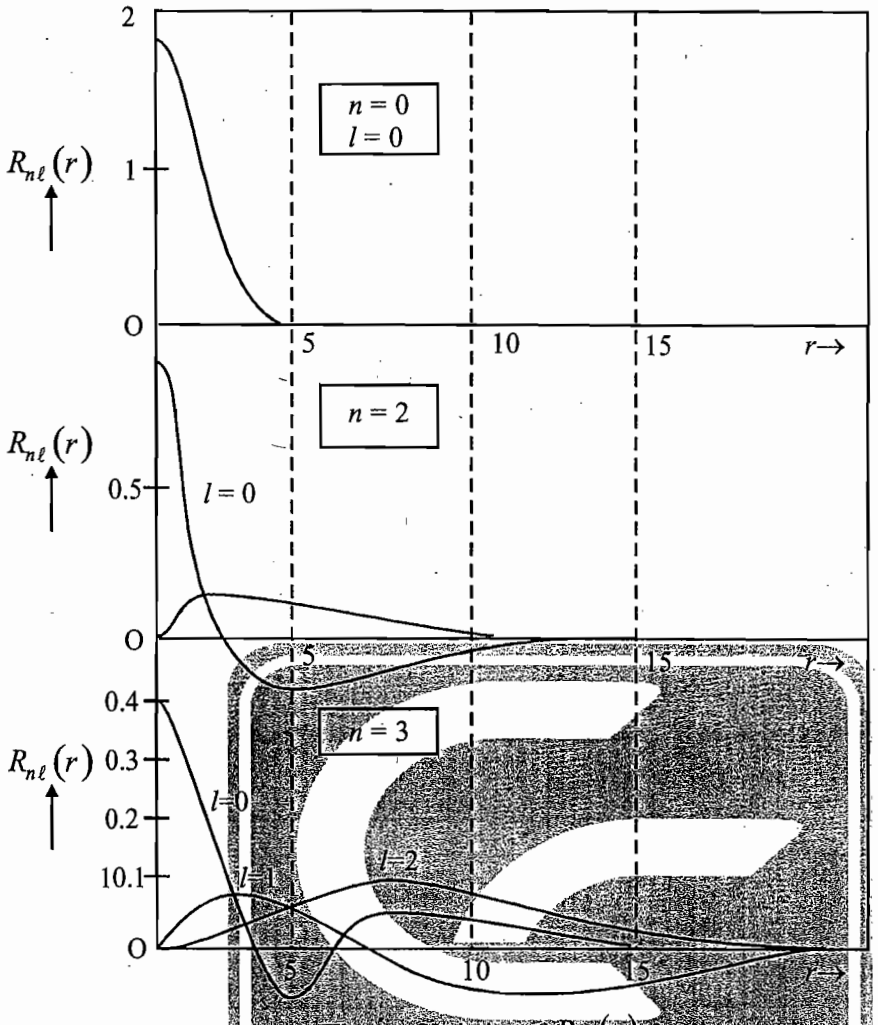

Figure : Variation of $R_{n\ell}(r)$ for various n with r.

Table : Real form of complete eigenfunction $\psi_{n\ell m}$ (excluding spin of the electron) for various values of n, l and m.

n	ℓ	m	State	$\psi_{n\ell m}$
1	0	0	$1s$	$\psi_{100} = \frac{1}{\sqrt{\pi}} \frac{1}{a_0^{3/2}} e^{-\rho/2}$
2	0	0	$2s$	$\psi_{200} = \frac{1}{4\sqrt{2\pi}} \frac{1}{a_0^{3/2}} (2-\rho) e^{-\rho/2}$
2	1	1	$2p$	$\psi_{211} = -\frac{1}{8\sqrt{\pi}} \frac{1}{a_0^{3/2}} \rho\, e^{-\rho/2} \sin\theta\, e^{i\phi}$
2	1	0	$2p$	$\psi_{210} = \frac{2}{4\sqrt{2\pi}} \frac{1}{a_0^{3/2}} \rho\, e^{-\rho/2} \cos\theta$
2	1	−1	$2p$	$\psi_{21-1} = \frac{1}{8\sqrt{\pi}} \frac{1}{a_0^{3/2}} \rho\, e^{-\rho/2} \sin\theta\, e^{-i\phi}$
3	0	0	$3s$	$\psi_{300} = \frac{1}{81\sqrt{3\pi}} \frac{1}{a_0^{3/2}} \left(27 - 18\rho + 2\rho^2\right) \times e^{-\rho/2}$

where, $\rho = \frac{2Z}{\quad}$, $a_0 = \frac{\hbar^2}{\quad}$

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Radial probability density :

The probability of finding the electron in volume element $d\tau$ is given by

$$|\psi_{nlm}|^2 d\tau = |\psi_{nlm}|^2 r^2 \sin\theta dr d\theta d\phi$$

Therefore, the probability of finding the electron in a spherical shell of radius r and thickness dr is,

$$P(r)dr = \int_{\theta=0}^{\pi}\int_{\phi=0}^{2\pi} |\psi_{nlm}|^2 r^2 \sin\theta dr d\theta d\phi = |R_{nl}|^2 r^2 dr$$

Here, $P(r)$ is called the radial probability density.

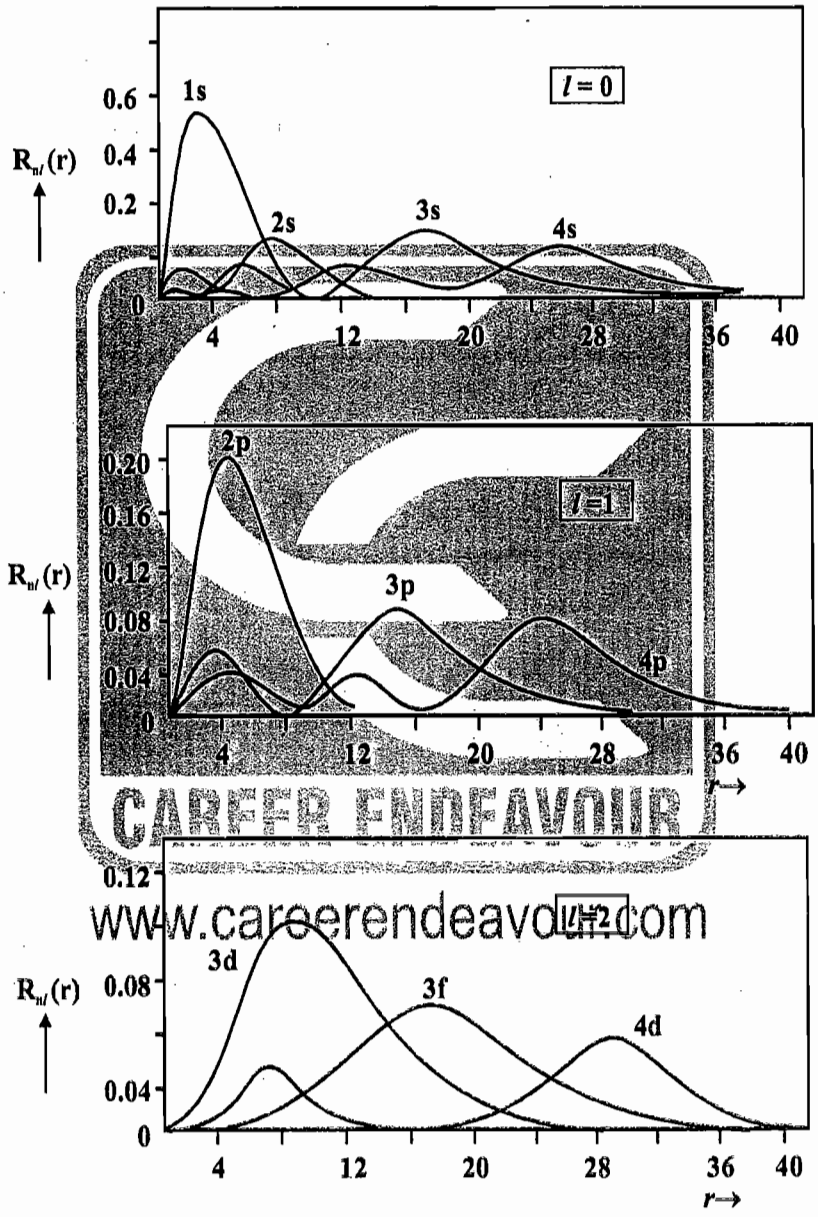

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Figure : Variation of $R_{n\ell}(r)$ with r in units of a_0

Energy values for the hydrogen atom:

Energy eigenvalues of n[th] state of hydrogen atom

$$E_n = -\frac{\mu z^2 e^4}{32\pi^2 \varepsilon_0^2 \hbar^2 n^2}$$

For the hydrogen atom $z = 1$ and hence

Sol

$$E_n = -\frac{\mu e^4}{32\pi^2\varepsilon_0^2\hbar^2 n^2} = -\frac{13.6}{n^2} eV$$

where, n = 1, 2, 3, ... and is called the principal quantum number.
This shows that the energy values for different quantum states discrete which is in agreement with old quantum theory and experiment.

Degeneracy:

For a particular value of $n, \ell = (n-1), (n-2), -2, -1, 0$, i.e. (n) values and for a particular value of l, $m = \ell, (\ell-1), (\ell-2), ..., 0, ..., -(\ell-1), -\ell$, i.e., $(2\ell+1)$ values. Thus degeneracy of a particular energy level is, $\sum_{l=0}^{n-1}(2l+1) = n^2$

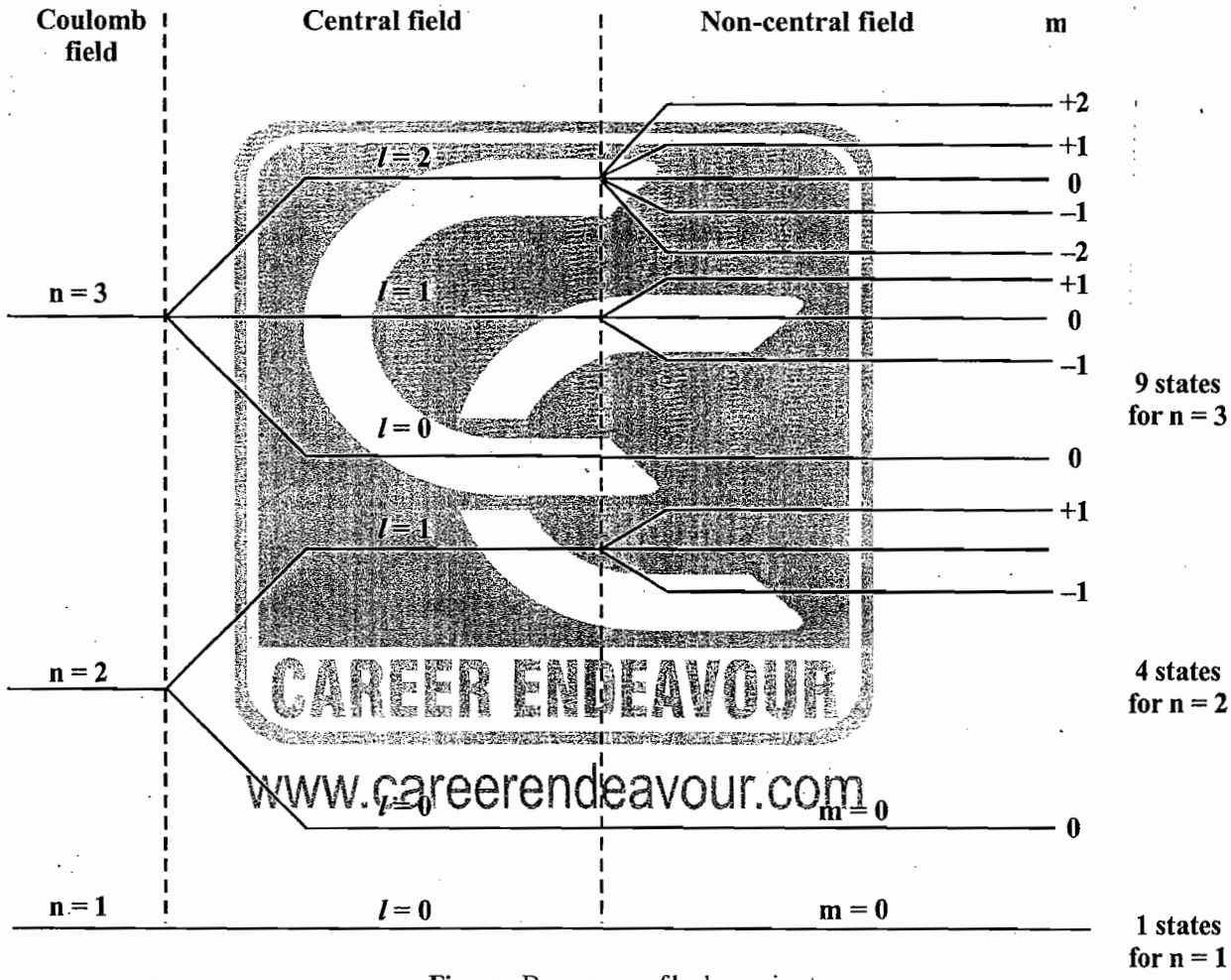

Figure : Degeneracy of hydrogenic atom

Example 6. Show that the most probable distance by the electron from the nucleus in the ground state of hydrogen atom is equal to the Bohr's radius.

Soln. For the ground state of hydrogen atom, $n = 1, \ell = 0$ and $m = 0$. Hence the ground state wave function is,

$$\psi_{1,0,0} = \left(\frac{1}{\pi a_0^3}\right)^{1/2} e^{-r/a_0}$$

Since, the wave function is independent of θ and ϕ, therefore,

Radial probability density = $P(r) = |\psi_{100}|^2 4\pi r^2 = \frac{4}{a_0^3} e^{-2r/a_0} r^2$

For most probable distance, $P(r)$ is to be the maximum

$$\frac{dP}{dr} = \frac{4}{a_0^3}\left[r^2\left(-\frac{2}{a_0}\right)e^{-2r/a_0} + 2re^{-2r/a_0}\right] = 0 \Rightarrow r = a_0$$

Thus the most probable distance of the electron from the nucleus of hydrogen atom in the ground state is equal tothe Bohr radius (a_0).

Example 7. The normalised ground state wave function of a one-electron atom is given by $\psi(r,\theta,\phi) = \pi^{-1/2}\left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0}$, where the notations have usual meaning. Evaluate the probability of the electron in this state will be found at a distance greater than $\frac{2a_0}{Z}$

Soln. The probability of finding the electron at a distance greater than $\frac{2a_0}{Z}$

$$P = \int_{2a_0/Z}^{\infty} \psi^*(r,\theta,\phi)\psi(r,\theta,\phi)4\pi r^2 dr = 4\pi \int_{2a_0/Z}^{\infty} |\psi|^2 r^2 dr$$

$$= 4\pi\int_0^{\infty} |\psi|^2 r^2 dr - 4\pi \int_0^{2a_0/Z} |\psi|^2 dr = 1 - 4\left(\frac{Z}{a_0}\right)^3 \int_0^{2a_0/Z} r^2 e^{-2Zr/a_0} dr$$

$$= 1 - 4\left(\frac{Z}{a_0}\right)^3 \left(\frac{a}{2Z}\right)^3 \int_0^2 \rho^2 e^{-\rho} d\rho \quad \left[\text{where, } \rho = \frac{2Z}{a_0} r\right]$$

$$= 1 - \frac{1}{2}\left(2 - 26e^{-2}\right) = 13e^{-2} = 0.15$$

Therefore, the probability of finding the electron in the normalised ground state of a one-electron atom at a distnce atom at a distance greater than $\frac{2a_0}{Z}$ from the nucleus is 15%.

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Example 8. If the ground state wave function for the hydrogen atom is

$$\psi = \frac{1}{\sqrt{\pi}} \frac{1}{a_0^{3/2}} e^{-r/a_0}$$

show that average distance of the electron from the nucleus is $1.5a_0$.

Soln. We have the average distance of the electron from the hydrogen nucleus in the ground state is,

$$\langle r \rangle = \int_0^{\infty} \psi^* \hat{r} \psi dr = \int_0^{\infty} \frac{1}{\sqrt{\pi}} \frac{1}{a_0^{3/2}} e^{-r/a_0} r \frac{1}{\sqrt{\pi}} \frac{1}{a_0^{3/2}} e^{-r/a_0} d\tau$$

$$= \frac{1}{\pi a_0^3} \int_0^{\infty} re^{-2r/a_0} r^2 \sin\theta dr d\theta d\phi$$

Using the standard integral $\int_0^\infty e^{-ax}x^n dx = \frac{n!}{a^{n+1}}$, we get

$$\langle r\rangle = \frac{1}{\pi a_0^3}\int_0^\infty r^3 e^{-2r/a_0}dr \int_0^\pi \sin\theta d\theta \int_0^{2\pi} d\phi = \frac{1}{\pi a_0^3}\times\frac{3!}{(2/a_0)^4}\times 2\times 2\pi$$

Therefore, $\langle r\rangle = \frac{3}{2}a_0 = 1.5a_0$

Example 9. Find the expectation value of potential energy of the electron in the hydrogen atom in the 1s state. The wave function for the electron is 1s state is given by

$$\psi_{1,0,0} = \frac{1}{\sqrt{\pi a_0^3}}e^{-r/a_0}$$

where, $a_0 = \frac{\hbar^2}{me^2}$ is the Bohr radius.

Soln. The potential energy of the electron in hydrogen atom is given by $V = -\frac{e^2}{r}$

Therefore, the expecgtation value of V is

$$V = +\int \psi_{1,0,0}^*\left(-\frac{e^2}{r}\right)\psi_{1,0,0}d\tau = -e^2\int|\psi_{1,0,0}|^2\frac{1}{r}d\tau$$

$$= -e^2\left(\frac{1}{\sqrt{\pi a_0^3}}\right)^2\int_0^\pi \sin\theta d\theta\int_0^{2\pi}d\phi\int_0^\infty \frac{e^{-2r/a_0}}{r}r^2dr$$

$$= -\frac{e^2}{\pi a_0^3}\times 4\pi\int_0^\infty e^{-2r/a_0}r\,dr = -\frac{me^4}{\hbar^2}$$

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Example 10. What is the expectation value of the kinetic energy (E_k) of the electron in the 1s state of the hydrogen atom?

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Soln. The expectation value of the kinetic energy is,

$$\langle E_k\rangle = \int_\tau \psi_{1,0,0}^*\,\hat{E}_k\psi_{1,0,0}d\tau = \int_0^\infty\int_0^\pi\int_0^{2\pi}\psi_{1,0,0}\hat{E}_k\psi_{1,0,0}r^2\sin\theta dr d\theta d\phi$$

But, $$\vec{E}_k = -\frac{\hbar^2}{2m}\nabla^2 = -\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}+\frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]$$

Since $\psi_{1,0,0}$ depends on r only, the terms in $\frac{\partial}{\partial\theta}$ and $\frac{\partial}{\partial\phi}$ are zero.

$$\therefore \quad \langle E_k\rangle = -\frac{\hbar^2}{2m}.4\pi\left(\frac{1}{\sqrt{\pi a_0^3}}\right)^2\int_0^\infty e^{-r/a_0}\times\left\{\left(\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}\right)e^{-r/a_0}\right\}r^2dr$$

$$= -\frac{\hbar^2}{2m}\frac{4}{a_0^3}\int_0^\infty \left(\frac{1}{a_0^2} - \frac{2}{ra_0}\right) e^{-2r/a_0} r^2 dr$$

$$= -\frac{2\hbar^2}{ma_0^3}\left[\frac{1}{a_0^2}\int_0^\infty r^2 e^{-2r/a_0} dr - \frac{2}{a_0}\int_0^\infty r e^{-2r/a_0} dr\right]$$

$$= -\frac{2\hbar^2}{ma_0^3}\left[\frac{1}{a_0^2}\frac{2}{(2/a_0)^3} - \frac{2}{a_0}\frac{1}{(2/a_0)^2}\right] = \frac{2\hbar^2}{ma_0^3}\cdot\frac{a_0}{4}$$

Therefore, $\langle E_k \rangle = \dfrac{\hbar^2}{2ma_0^3} = \dfrac{\hbar^2}{2m}\left(\dfrac{me^2}{\hbar^2}\right) = \dfrac{me^4}{2\hbar^2}$

Example 11. Estimate the uncertainity in the radial position of the electron in the ground state of hydrogen atom.

Soln. For ground state, $\langle r \rangle = \dfrac{4}{a_0^3}\int_0^\infty r^3 \exp\left(\dfrac{-2r}{a_0}\right) dr = \dfrac{3a_0}{2}$

$$\langle r^2 \rangle = \frac{4}{a_0^3}\int_0^\infty r^4 \exp\left(\frac{-2r}{a_0}\right) dr = 3a_0^2$$

Uncertainity in the radial position of the particle will be

$$\Delta r = \sqrt{\langle r^2 \rangle - \langle r \rangle^2} = \frac{\sqrt{3}}{2} a_0$$

Example 12. Find out the positions of maxima of the radial probability curves for $1s$, $2p$ and $3d$ orbitals of a hydrogen-like atom.

Soln. The radial probability density $P_{nl} = r^2 |R_{nl}|^2$. Then,

$$R_{10} = \text{constant} \times \exp\left(-\frac{Zr}{a_0}\right), R_{21} = \text{constant} \times r \exp\left(-\frac{Zr}{2a_0}\right), R_{32} = \text{constant} \times r \exp\left(-\frac{Zr}{3a_0}\right)$$

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P_{nl} will be maximum when $dP_{nl}/dr = 0$, and hence

$$\frac{dP_{10}}{dr} = 0 = \text{constant}\left(2r - \frac{2Zr^2}{a_0}\right)\exp\left(-\frac{2Zr}{a_0}\right), \; r = \frac{a_0}{Z}$$

$$\frac{dP_{21}}{dr} = 0 = \text{constant}\left(4r^3 - \frac{Zr^4}{a_0}\right)\exp\left(-\frac{Zr}{a_0}\right), \; r = \frac{4a_0}{Z}$$

Similarly, $dP_{32}/dr = 0$ gives $r = 9a_0/Z$

In general, $r_{\max} = n^2 a_0 / Z$

Example 13. A positron and an electron form a shortlived atom called positronium before the two annihilate to produce gamma rays. Calculate, in electron volts, the ground state energy of positronium.

Soln. The positron has a charge $+e$ and mass equal to the electron mass.

Reduced mass for the positronium atom, is

$$\frac{m_e.m_e}{2m_e}=\frac{m_e}{2}$$

where m_e is the electron mass.

Since, the energy for the hydrogen like atoms is directly proportional to the reduced mass. Therefore, energy of the positronium atom is half the energy of hydrogen atom.

Therefore, the ground state energy for the positronium atom is $-\frac{13.6}{2}eV=-6.8eV$

Example 14. At time $t = 0$, the wave function for the hydrogen atom is

$$\psi(r,0)=\frac{1}{\sqrt{10}}(2\psi_{100}+\psi_{210}+\sqrt{2}\psi_{211}+\sqrt{3}\psi_{21,-1})$$

where the subscripts are values of the quantum numbers n, l, m. (i) What is the expectation value for the energy of the system? (ii) What is the probability of finding the system with $l = 1$, $m = 1$?

Soln. (i) The expectation value of the energy of the system

$$\langle E\rangle=\langle\psi|H|\psi\rangle$$

$$=\frac{1}{10}\left\langle(2\psi_{100}+\psi_{210}+\sqrt{2}\psi_{211}+\sqrt{3}\psi_{21,-1})|H|(2\psi_{100}+\psi_{210}+\sqrt{2}\psi_{211}+\sqrt{3}\psi_{21,-1})\right\rangle$$

$$=\frac{1}{10}\left\langle(2\psi_{100}+\psi_{210}+\sqrt{2}\psi_{211}+\sqrt{3}\psi_{21,-1})|(2E_1\psi_{100}+E_2\psi_{210}+\sqrt{2}E_2\psi_{211}+\sqrt{3}E_2\psi_{21,-1})\right\rangle$$

$$=\frac{1}{10}(4E_1+E_2+2E_2+3E_2)=\frac{1}{10}(4E_1+6E_2)$$

Since $E_1 = -13.8$ eV and $E_2 = -3.4$ eV,

$$\langle E\rangle=\frac{1}{10}(-54.4\text{eV}-20.4\text{eV})=-7.48\text{eV}$$

(ii) The required probability is given by $P=\frac{2}{10}\langle 211|211\rangle=\frac{2}{10}=\frac{1}{5}$

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CSIR PREVIOUS YEAR QUESTIONS

1. The energy levels of the non-relativistic electron in a hydrogen atom (i.e. in a Coulomb potential $V(r) \propto -1/r$ are given by $E_{n\ell m} \propto -1/n^2$, where n is the principal quantum number, and the corresponding wave functions are given by $\psi_{n\ell m}$, where ℓ is the orbital angular momentum quantum number and m is the magnetic quantum number. The spin of the electron is not considered. Which of the following is a correct statement? **[CSIR June 2011]**

(a) There are exactly $(2\ell+1)$ different wave functions $\psi_{n\ell m}$, for each $E_{n\ell m}$.

(b) There are $\ell(\ell+1)$ different wave functions $\psi_{n\ell m}$, for each $E_{n\ell m}$.

(c) $E_{n\ell m}$ does not depend on ℓ and m for the Coulomb potential.

(d) There is a unique wave function $\psi_{n\ell m}$ and $E_{n\ell m}$.

Soln. Energy eigenvalues of the n^{th} state of a hydrogen atom $E_n = -\dfrac{13.6\ eV}{n^2}$

The energy E_n depends only on n and not on ℓ and m. This is due to the degeneracy n^2 (neglecting spin) that arises due to the spherical symmetry of the Columb potential which depends only on radial distance 'r' of the electron from the nucleus.

Correct answer is (c).

2. If an electron is in the ground state of the hydrogen atom, the probability that its distance from the proton is more than one Bohr radius is approximately. **[CSIR June 2011]**

(a) 0.68 (b) 0.48 (c) 0.28 (d) 0.91

Soln. Ground state wave function of the particle $\psi_{100}(r) = \dfrac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}$

Probability for electron to lie between a_0 to ∞ is:

$$P = \int_{a_0}^{\infty} |\psi_{100}(r)|^2 4\pi r^2 dr = \frac{4}{a_0^3}\int_{a_0}^{\infty} r^2 e^{-2r/a_0} dr = \frac{5}{e^2} = 0.68$$

Correct answer is (a)

3. Given that the ground state energy of the hydrogen atom is -13.6 eV, the ground state energy of positronium (which is a bound state of an electron and a positron) is **[CSIR Dec 2011]**

(a) 6.8 eV (b) -6.8 eV (c) -13.6 eV (d) -27.2 eV

Soln. For positronium atom, reduced mass $\mu = \dfrac{m_e m_e^+}{m_e + m_e^+} = \dfrac{m_e}{2}$

Since the energy eigenvalues of hydrogen like atoms is proportional to reduced mass μ of the system.

Therefore, energy of the positronium atom $E_p = \dfrac{E_H}{2} = -\dfrac{6.8}{n^2} eV$

Ground state energy of the positronium atom $E_{p,0} = -\dfrac{1}{2} \times \dfrac{13.6}{1^2} = -6.8\ eV$

Correct answer is (b).

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4. The energy of the first excited quantum state of a particle in the two-dimensional potential $V(x,y)=\frac{1}{2}m\omega^2\left(x^2+4y^2\right)$ is: **[CSIR Dec 2011]**

(a) $2\hbar\omega$ (b) $3\hbar\omega$ (c) $\frac{3}{2}\hbar\omega$ (d) $\frac{5}{2}\hbar\omega$

Soln. Given potential: $V(x,y)=\frac{1}{2}m\omega^2x^2+\frac{1}{2}m(2\omega)^2y^2$

Energy eigenvalue $E_n=\left(n_x+\frac{1}{2}\right)\hbar\omega+\left(n_y+\frac{1}{2}\right)\hbar\times2\omega$

Ground state: $n_x=0,\ n_y=0;\qquad E_0=\frac{3}{2}\hbar\omega$

First excited state: $n_x=1, n_y=0;\qquad E_1=\frac{3}{2}\hbar\omega+\frac{1}{2}\hbar\times2\omega=\frac{5}{2}\hbar\omega$

Correct answer is (d)

5. A particle of mass m is in a cubic box of size a. The potential inside the box. $(0\le x<a, 0\le y<a, 0\le z<a)$ is zero and infinte outside. If the particle is in an eigenstate of energy $E=\frac{14\pi^2h^2}{2ma^2}$, its wave function is: **[CSIR June 2012]**

(a) $\psi=\left(\frac{2}{a}\right)^{3/2}\sin\frac{3\pi x}{a}\sin\frac{5\pi y}{a}\sin\frac{6\pi z}{a}$ (b) $\psi=\left(\frac{2}{a}\right)^{3/2}\sin\frac{7\pi x}{a}\sin\frac{4\pi y}{a}\sin\frac{3\pi z}{a}$

(c) $\psi=\left(\frac{2}{a}\right)^{3/2}\sin\frac{4\pi x}{a}\sin\frac{8\pi y}{a}\sin\frac{2\pi z}{a}$ (d) $\psi=\left(\frac{2}{a}\right)^{3/2}\sin\frac{\pi x}{a}\sin\frac{2\pi y}{a}\sin\frac{3\pi z}{a}$

Soln. The energy of the particle in cubic box of size a is $=\frac{\hbar^2\pi^2}{2ma^2}\left(n_x^2+n_y^2+n_z^2\right)$, n_X, n_Y, and n_Z= 1, 2, 3, 4....

For energy $E=\frac{14\hbar^2\pi^2}{2ma^2}$, the possible values of $(n_x,n_y,n_z)=(1,2,3),(1,3,2),(2,1,3),(2,3,1),(3,1,2),(3,2,1)$

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The wave function the particle $\psi_n=\left(\sqrt{\frac{2}{a}}\right)^3\sin\left(\frac{n_x\pi x}{a}\right)\sin\left(\frac{n_y\pi y}{a}\right)\sin\left(\frac{n_z\pi z}{a}\right)$

On substituting (1,2,3) in place of (n_X, n_Y, n_Z), we get $\psi=\left(\frac{2}{a}\right)^{3/2}\sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{2\pi y}{a}\right)\sin\left(\frac{3\pi z}{a}\right)$

Correct answer is (d)

6. Let $\Psi_{n\ell m}$ denote the eigenfunctions of a Hamiltonian for a spherically symmetric potential V(r). The wavefunction $\Psi=\frac{1}{4}\left[\Psi_{210}+\sqrt{5}\Psi_{21-1}+\sqrt{10}\Psi_{213}\right]$ is an eigenfunction of **[CSIR June 2012]**

(a) H, L^2 and L_z (b) H and L_z (c) H and L^2 (d) L^2 and L_z

Soln. The wavefunction $\psi = \frac{1}{4}\left[\psi_{210} + \sqrt{5}\,\psi_{21-1} + \sqrt{10}\,\psi_{211}\right]$

For spherically symmetric potential $H\psi_{nlm} = E_n\,\psi_{n\ell m}$, where E_n depends only an n and independent of l and m.

$$L^2\psi_{nlm} = \ell(\ell+1)\hbar^2\psi_{nlm};\ L_z\,\psi_{n\ell m} = m\hbar\,\psi_{n\ell m}$$

$$H\psi = \frac{1}{4}\left[H\psi_{210} + \sqrt{5}\,H\psi_{21-1} + \sqrt{10}\,H\psi_{211}\right]$$

$$= \frac{E_2}{4}\left[\psi_{210} + \sqrt{5}\psi_{21-1} + \sqrt{10}\psi_{211}\right] = E_2\psi$$

So ψ is an eigen function of H corresponding to eigenvalue E_2.

$$L^2\psi = \frac{1}{4}\left[L^2\psi_{210} + \sqrt{5}L^2\psi_{21-1} + \sqrt{10}L^2\psi_{211}\right]$$

$$= \frac{1}{4}\left[\left(2\hbar^2\right)\psi_{210} + \sqrt{5}\left(2\hbar^2\right)\psi_{21-1} + \sqrt{10}\left(2\hbar^2\right)\psi_{211}\right] = 2\hbar^2\psi$$

So ψ is an eigen function of L^2 corresponding to eigenvalue $2\hbar^2$.

$$L_z\psi = \frac{1}{4}\left[L_z\psi_{210} + \sqrt{5}\,L_z\psi_{21-1} + \sqrt{10}\,L_z\psi_{211}\right]$$

$$= \frac{1}{4}\left[0\times\psi_{210} + \sqrt{5}(-\hbar)\psi_{21-1} + \sqrt{10}(\hbar)\psi_{211}\right] \neq L_z\psi$$

So ψ is not an eigen function of L_z.

Correct answer is (c)

7. The wave function of a state of the hydrogen atom is given by

$$\psi = \psi_{200} + 2\psi_{211} + 3\psi_{210} + \sqrt{2}\,\psi_{21-1}$$

where $\psi_{n\ell m}$ denotes the normalized eigen function of the state with quantum numbers n, l and m in the usual notation. The expectation value of L_z in the state ψ is: **[CSIR Dec 2012]**

(a) $\frac{15\hbar}{16}$ (b) $\frac{11\hbar}{16}$ (c) $\frac{3\hbar}{8}$ (d) $\frac{\hbar}{8}$

Soln. The given wavefunction is $\psi = \frac{1}{4}\psi_{200} + \frac{1}{2}\psi_{211} + \frac{3}{4}\psi_{210} + \frac{\sqrt{2}}{4}\psi_{21-1}$

where $\psi_{n\ell m}$ denotes the normalized eigen function of L_z corresponding to eigenvalue $m_l\hbar$.

Normalized form of the given wavefunction is

$$\psi = \frac{1}{4}\psi_{200} + \frac{1}{2}\psi_{211} + \frac{3}{4}\psi_{210} + \frac{\sqrt{2}}{4}\psi_{21-1}$$

The expectation value of L_z is

$$\langle L_z\rangle = \sum_\ell |C_\ell|^2\, m_\ell\hbar = \frac{1}{16}(0\hbar) + \frac{4}{16}(1\hbar) + \frac{9}{16}(0\hbar) + \frac{2}{16}(-1\hbar) = \frac{\hbar}{8}$$

Correct answer is (d)

8. The un-normalized wavefunction of a particle in a spherically symmetric potential is given by $\psi(\vec{r}) = zf(r)$ where f(r) is a function of the radial variable r. The eigenvalue of the operator $\vec{L}^2$ (namely the square of the orbital angular momentum) is **[CSIR June 2013]**

(a) $\hbar^2/4$ (b) $\hbar^2/2$ (c) $\hbar^2$ (d) $2\hbar^2$

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Soln. The un-normalized wavefunction $\psi(\vec{r}) = Z\, f(r)$

In spherical polar co-ordinate system

$$\psi(\vec{r}) = r\cos\theta\, f(r)$$

$\psi(\vec{r})$ has only power of $\cos\theta$ so the orbital quantum number $\ell = 1$

The eigenvalue of $L^2 = \ell(\ell+1)\hbar^2 = 2\hbar^2$

Correct answer is (d)

9. If ψ_{nlm} denotes the eigenfunction of the Hamiltonian with a potential V = V(r) then the expectation value of the operator $L_x^2 + L_y^2$ in the state $\psi = \frac{1}{5}[3\psi_{211} + \psi_{210} - \sqrt{15}\psi_{21-1}]$ is

[CSIR June 2013]

(a) $39\hbar^2/25$ (b) $13\hbar^2/25$ (c) $2\hbar^2$ (d) $26\hbar^2/25$

Soln. $\psi = \frac{1}{5}\left[3\psi_{211} + \psi_{210} - \sqrt{15}\psi_{21-1}\right]$

$$|\psi\rangle = \frac{1}{5}\left[3|\psi_{211}\rangle + |\psi_{210}\rangle - \sqrt{15}|\psi_{21-1}\rangle\right]$$

$$\langle\psi| = \frac{1}{5}\left[3\langle\psi_{211}| + \langle\psi_{210}| - \sqrt{15}\langle\psi_{21-1}|\right]$$

The expectation value of the operator

$$\left\langle\left(L_x^2 + L_y^2\right)\right\rangle = \left\langle L^2 + L_y^2 + L_z^2 - L_z^2\right\rangle = \left\langle L^2 - L_z^2\right\rangle = \left\langle L^2\right\rangle - \left\langle L_z^2\right\rangle \quad \ldots (1)$$

$$\left\langle L^2\right\rangle = \left\langle\psi\left|L^2\right|\psi\right\rangle$$

$$= \frac{1}{5}\left[\langle\psi_{211}|3 + \langle\psi_{210}| - \sqrt{15}\langle\psi_{21-1}|\right]\frac{1}{5}\left[3L^2|\psi_{211}\rangle + L^2|\psi_{210}\rangle - \sqrt{15}L^2|\psi_{21-1}\rangle\right]$$

$$= \frac{1}{25}\left[\langle\psi_{211}|3 + \langle\psi_{210}| - \sqrt{15}\langle\psi_{21-1}|\right]\left[3\times 2\hbar^2|\psi_{211}\rangle + 2\hbar^2|\psi_{210}\rangle - \sqrt{15}2\hbar^2|\psi_{21-1}\rangle\right]$$

$$= \frac{3\times 3}{25}\times 2\hbar^2 + \frac{1}{25}\times 2\hbar^2 + \frac{15}{25}\times 2\hbar^2 = 2\hbar^2 \qquad [\text{Using } \langle n\ell'm'|n\ell m\rangle = \delta_{\ell\ell'}\delta_{mm'}]$$

$$\left\langle L_z^2\right\rangle = \left\langle\psi\left|L_z^2\right|\psi\right\rangle$$

$$= \frac{1}{25}\left[\langle\psi_{211}|3 + \langle\psi_{210}| - \langle\psi_{21-1}|\sqrt{15}\right]\left[3L_z^2|\psi_{211}\rangle + L_z^2|\psi_{210}\rangle - \sqrt{15}L_z^2|\psi_{21-1}\rangle\right]$$

$$= \frac{1}{25}\left[\langle\psi_{211}|3 + \langle\psi_{210}\rangle - \langle\psi_{211} - 1|\sqrt{15}\right]\left[3\hbar^2\langle\psi_{211}| + 0 - \sqrt{15}\,\hbar^2|\psi_{21-1}\rangle\right]$$

$$= \left(\frac{9}{25} + \frac{15}{25}\right)\hbar^2 = \frac{24}{25}\hbar^2$$

On substituting the values of $\left\langle L^2\right\rangle$ and $\left\langle L_z^2\right\rangle$ in equation (i), we get

$$\left\langle\left(L_x^2 + L_y^2\right)\right\rangle = 2\hbar^2 - \frac{24}{25}\hbar^2 = \frac{26}{25}\hbar^2$$

Correct answer is (d)

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10. A particle of mass m in three dimensions is in the potential

$$V(r)=\begin{cases}0 & r<a\\ \infty & r\geq a\end{cases}$$

Its ground state energy is **[CSIR June 2014]**

(a) $\frac{\pi^2\hbar^2}{2ma^2}$ (b) $\frac{\pi^2\hbar^2}{ma^2}$ (c) $\frac{3\pi^2\hbar^2}{2ma^2}$ (d) $\frac{9\pi^2\hbar^2}{2ma^2}$

Soln. The energy eigenvalues of the given infinite spherical square well potential is

$$E_n=\frac{n^2\pi^2\hbar^2}{2ma^2} \quad \text{for } \ell=0 \qquad (n=1,2,3,.....)$$

The ground state energy will be $\frac{\pi^2\hbar^2}{2ma^2}$

Correct answer is (a)

11. Given that $\hat{p}_r=-i\hbar\left(\frac{\partial}{\partial r}+\frac{1}{r}\right)$, the uncertainty Δp_r in the ground state

of the hydrogen atom is $\psi_0(r)=\frac{1}{\sqrt{\pi a_0^3}}e^{-r/a_0}$ **[CSIR June 2014]**

(a) $\frac{\hbar}{a_0}$ (b) $\frac{\sqrt{2}\hbar}{a_0}$ (c) $\frac{\hbar}{2a_0}$ (d) $\frac{2\hbar}{a_0}$

Soln. $\hat{p}_r=-i\hbar\left(\frac{\partial}{\partial r}+\frac{1}{r}\right)$

$$\hat{p}_r^2=(-i\hbar)^2\left(\frac{\partial}{\partial r}+\frac{1}{r}\right)\left(\frac{\partial}{\partial r}+\frac{1}{r}\right)=-\hbar^2\left(\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}\right)$$

Given : Ground state wave function $\psi_0=\frac{1}{\sqrt{\pi a_0^3}}e^{-r/a_0}$

$\langle\hat{p}_r\rangle=\langle\psi_0|\hat{p}_r|\psi_0\rangle=0$ (since the wave function is real)

$$\langle\hat{p}_r^2\rangle=\int_0^\infty\frac{1}{\sqrt{\pi a_0^3}}e^{-r/a_0}\left(-\hbar^2\left(\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}\right)\left(\frac{1}{\sqrt{\pi a_0^3}}e^{-r/a_0}\right)\right)4\pi r^2dr$$

$$=\int_0^\infty\frac{1}{\pi a_0^3}\left(-\hbar^2\right)e^{-r/a_0}\left[\frac{1}{a_0^2}e^{-r/a_0}+\frac{2}{r}\left(-\frac{1}{a_0}\right)e^{-r/a_0}\right]4\pi r^2dr$$

$$=-\frac{\hbar^2 4\pi}{\pi a_0^3}\left[\frac{1}{a_0^2}\int_0^\infty e^{-2r/a_0}r^2dr-\frac{2}{a_0}\int_0^\infty e^{-2r/a_0}.rdr\right]$$

Using the integration : $\int_0^\infty e^{-ar}r^n dr=\frac{n!}{a^{n+1}}$

$$=-\frac{4\hbar^2}{a_0^3}\left[\frac{1}{a_0^2}\frac{2!}{(2/a_0)^3}-\frac{2}{a_0}\frac{1!}{(2/a_0)^2}\right]=-\frac{4\hbar^2}{a_0^3}\left[\frac{a_0}{4}-\frac{a_0}{2}\right]=\frac{\hbar^2}{a_0^2}$$

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Momentum spread $= \Delta\hat{p}_r = \sqrt{\langle \hat{p}_r^2 \rangle - \langle \hat{p}_r \rangle^2} = \frac{\hbar}{a_0}$

Correct answer is (a)

)14]

12. A particle of mass m in the potential $V(x,y) = \frac{1}{2}m\omega^2\left(4x^2 + y^2\right)$, is in an eigenstate of energy $E = \frac{5}{2}\hbar\omega$. The corresponding un-normalized eigenfunction is **[CSIR June 2014]**

(a) $y\exp\left[-\frac{m\omega}{2\hbar}\left(2x^2 + y^2\right)\right]$ (b) $x\exp\left[-\frac{m\omega}{2\hbar}\left(2x^2 + y^2\right)\right]$

(c) $y\exp\left[-\frac{m\omega}{2\hbar}\left(x^2 + y^2\right)\right]$ (d) $xy\exp\left[-\frac{m\omega}{2\hbar}\left(x^2 + y^2\right)\right]$

Soln. $V(x,y) = \frac{1}{2}m\omega^2\left(4x^2 + y^2\right) = \frac{1}{2}m(2\omega)^2 x^2 + \frac{1}{2}m(\omega)y^2$

It is a 2-D anisotropic harmonic oscillator having $\omega_x = 2\omega$ and $\omega_y = \omega$

Energy eigenvalue $= E_{n_x n_y} = \left(n_x + \frac{1}{2}\right)\hbar(2\omega) + \left(n_y + \frac{1}{2}\right)\hbar(\omega) = \left(n + \frac{3}{2}\right)\hbar\omega$ (where, $n = 2n_x + n_y$)

)14] Given: $E_{n_x n_y} = \frac{5}{2}\hbar\omega \Rightarrow n_x = 0, n_y = 1$

The corresponding wavefunction will be,

$\psi_{n_x n_y}(x,y) = A_x e^{-\alpha_x^2 x^2/2} H_{n_x}(\alpha_x x).A_y e^{-\alpha_y^2 y^2/2} H_{n_y}(\alpha_y y)$ where, $\alpha_x^2 = \frac{m(2\omega)}{\hbar}, \alpha_y^2 = \frac{m(\omega)}{\hbar}$

$\psi_{01}(x,y) = A_x A_y H_0(\alpha_x x).H_1(\alpha_y y).\exp\left[-\frac{1}{2}\left(\alpha_x^2 x^2 + \alpha_y^2 y^2\right)\right]$

$\Rightarrow \quad \psi_{01}(x,y) = A_x A_y (1)(2\alpha_y y)\exp\left[-\frac{m\omega}{2\hbar}\left(2x^2 + y^2\right)\right]$

Correct answer is (a)

13. An electron is in the ground state of a hydrogen atom. The probability that it is within the Bohr radius is approximately equal to **[CSIR June 2014]**

(a) 0.60 (b) 0.90 (c) 0.16 (d) 0.32

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Soln. Probability that the electron will be within the Bohr radius

$= \int_0^{a_0} \psi_0^* \psi_0 4\pi r^2 dr$, where, $\psi_0 = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}$

$= \frac{1}{\pi}\frac{4\pi}{a_0^3}\int_0^{a_0} e^{-2r/a_0} . r^2 dr = 1 - \frac{5}{e^2} = 0.32$

Correct answer is (d)

PRACTICE SET

1. The spinless particle moves in a central potential $V(r)$. Which of the following statement is TRUE? **[GATE 2001]**

(a) The kinetic energy and the potential energy of the particle cannot have simultanous sharp values.
(b) The total energy and the potential energy of the particle can have simultanous sharp values.
(c) The total energy and the square of the orbital angular momentum about the origin cannot have simultanous sharp values.
(d) The total energy of the particle can have only discrete eigenvalues.

2. A quantum particle of mass m is confined to a square region in xy-plane whose vertices are given by (0, 0), (L, 0), (L, L) and (0, L). Which of the following represents an admissible wave function of the particle (for l, m, n positive integers)? **[GATE 2001]**

(a) $\frac{2}{L}\sin\left(\frac{n\pi x}{L}\right)\cos\left(\frac{m\pi y}{L}\right)$ (b) $\frac{2}{L}\sin\left(\frac{\ell\pi x}{L}\right)\cos\left(\frac{n\pi y}{L}\right)$

(c) $\frac{2}{L}\sin\left(\frac{m\pi x}{L}\right)\sin\left(\frac{n\pi y}{L}\right)$ (d) $\frac{2}{L}\cos\left(\frac{n\pi x}{L}\right)\sin\left(\frac{\ell\pi y}{L}\right)$

Common data for Q.3 and Q.4
A particle is located in a three diamensional cubic well of width L with impenetrable walls **[GATE 2003]**

3. The sum of he energies of the third and the fourth levels is:

(a) $10\pi^2\hbar^2/mL^2$ (b) $10\pi^2\hbar^2/3\,mL^2$ (c) $11\pi^2\hbar^2/2mL^2$ (d) $5\pi^2\hbar^2/2mL^2$

4. The degeneracy of the fourth level is given by

(a) 1 (b) 2 (c) 3 (d) 4

5. In a hydrogen atom, the accidental or Coulomb degenaracy for the n = 4 state is **[GATE 2004]**

(a) 4 (b) 16 (c) 18 (d) 32

6. The expectation value of the z coordinate (z), in the ground state of the hydrogen atom (wavefunction: $\psi_{100}(r) = Ae^{-r/a_0}$, where A is the normalization constant and a_0 is the Bohr radius), is **[GATE 2005]**

(a) a_0 (b) $\frac{a_0}{2}$ (c) $\frac{a_0}{4}$ (d) 0

7. The degeneracy of the n = 2 level for a three dimensional isotropic oscillator is **[GATE 2005]**

(a) 4 (b) 6 (c) 8 (d) 10

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8. A particle is moving in a spherically symmetric potential $V(r) = \alpha r^2$, where α is a postive constant. In a stationary state, the expectation value of the kinetic energy of the particle is **[GATE 2006]**

(a) $\langle T\rangle = \langle V\rangle$ (b) $\langle T\rangle = 2\langle V\rangle$ (c) $\langle T\rangle = 3\langle V\rangle$ (d) $\langle T\rangle = 4\langle V\rangle$

9. An atomic state of hydrogen is represented by the following wave function:

$$\psi(r,\theta,\phi) = \frac{1}{\sqrt{2}}\left(\frac{1}{a_0}\right)^{3/2}\left(1-\frac{r}{2a_0}\right)e^{-r/2a_0}\cos\theta$$

where a_0 is a constant. The quantum number of the state are **[GATE 2007]**

(a) $\ell = 0, m = 0, n = 1$ (b) $\ell = 1, m = 1, n = 2$ (c) $\ell = 1, m = 0, n = 2$ (d) $\ell = 2, m = 0, n = 3$

10. The radial wave function of the electrons in the state of n = 1 and l = 0 in a hydrogen atom is $R_{10} = \frac{2}{a_0^{3/2}} \exp\left(-\frac{r}{a_0}\right)$, a_0 is the Bohr radius. The most probable value of r for an electron is:

[GATE 2008]

(a) a_0 (b) $2a_0$ (c) $4a_0$ (d) $8a_0$

11. The normalized ground state wavefunction of a hydrogen atom is given by $\psi(r) = \frac{1}{\sqrt{4\pi}} \frac{2}{a^{3/2}} e^{-r/a}$, where a is the Bohr radius and r is the distance of the electron from the nucleus, located at the origin. The expectation value $\left\langle \frac{1}{r^2} \right\rangle$ is:

[GATE 2011]

(a) $\frac{8\pi}{a^2}$ (b) $\frac{4\pi}{a^2}$ (c) $\frac{4}{a^2}$ (d) $\frac{2}{a^2}$

12. A particle of mass m is confined in a two dimensional square well potential of dimension a. This potential $V(x, y)$ is given by

$V(x, y) = 0$ for $0 < x < a$ and $0 < y < a$

$= \infty$ else where

The energy of the first excited state for this particle is given by:

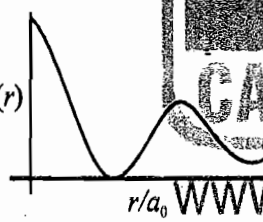
[GATE 2012]

(a) $\frac{\pi^2\hbar^2}{ma^2}$ (b) $\frac{2\pi^2\hbar^2}{ma^2}$ (c) $\frac{5\pi^2\hbar^2}{2ma^2}$ (d) $\frac{4\pi^2\hbar^2}{ma^2}$

13. The ground state wavefunction for the hydrogen atom is given by $\psi_{100} = \frac{1}{\sqrt{4\pi}} \left(\frac{1}{a_0}\right)^{3/2} e^{-r/a_0}$, where a_0 is the Bohr radius. The plot of the radial probability density, P(r) for the hydrogen atom in the ground state is

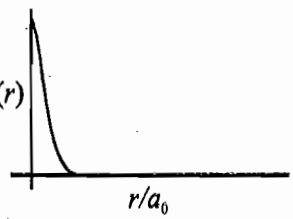
[GATE 2012]

(a)

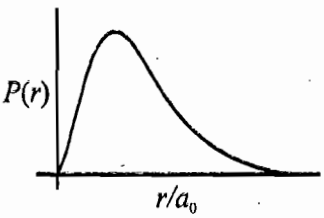


(b)

(c)



(d)



14. An electron in the ground state of the hydrogen atom has the wave function

$$\psi(\vec{r}) \frac{1}{\sqrt{\pi a_0^3}} e^{-(r/a_0)}$$

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where a_0 is constant. The expectation value of the operator $\hat{Q} = z^2 - r^2$, where $z = r\cos\theta$ is (Hint: $\int_0^\infty e^{-ar} r^n dr = \frac{\Gamma(n)}{\alpha^{n+1}} = \frac{(n-1)!}{\alpha^{n+1}}$) **[GATE 2014]** (a)

$-\frac{a_0^2}{2}$ (b) $-a_0^2$ (c) $-\frac{3a_0^2}{2}$ (d) $-2a_0^2$

15. A particle of mass 'm' is subjected to a potential, **[GATE 2014]**

$$V(x,y) = \frac{1}{2}m\omega^2\left(x^2 + y^2\right), \quad -\infty \le x \le \infty, -\infty \le y \le \infty$$

The state with energy $4\hbar\omega$ is g-fold degenerate. The value of g is _____

16. A hydrogen atom is in the state

$$\psi = \sqrt{\frac{8}{21}}\psi_{200} - \sqrt{\frac{3}{7}}\psi_{310} + \sqrt{\frac{4}{21}}\psi_{321}$$ **[GATE 2014]**

where n, ℓ, m in $\psi_{n\ell m}$ denote the principal, orbital and magnetic quantum numbers, respectively. If $\vec{L}$ is the angular momentum operator, the average value of L^2 is _____ $\hbar^2$

17. The normalized wavefunctions of a Hydrogen atom are denoted by $\psi_{n,\ell,m}(\vec{x})$, where n, ℓ and m are, respectively, the principal, azimuthal and magnetic quantum numbers respectively. Now consider an electron in the mixed state

$$\Psi(\vec{x}) = \frac{1}{3}\psi_{1,0,0}(\vec{x}) + \frac{2}{3}\psi_{2,1,0}(\vec{x}) + \frac{2}{3}\psi_{3,2,-2}(\vec{x})$$ **[TIFR 2012]**

The expectation value $\langle E \rangle$ of the energy of this electron, in electron-Volts (eV) will be approximately

(a) –1.5 (b) –3.7 (c) –13.6 (d) –80.1

(e) +13.6

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18. An energy eigenstate of the Hydrogen atom has the wave function

$$\psi_{n\ell m}(r,\theta,\varphi) = \frac{1}{81\sqrt{\pi}}\left(\frac{1}{a_0}\right)^{3/2} \sin\theta\cos\theta\exp\left[-\left(\frac{r}{3a_0} + i\varphi\right)\right]$$ **[TIFR 2013]**

where a_0 is the Bohr radius. The principal (n), azimuthal (ℓ) and magnetic (m) quantum numbers corresponding to this wave function are

(a) $n = 3, \ell = 2, m = 1$ (b) $n = 2, \ell = 1, m = 1$

(c) $n = 3, \ell = 2, m = -1$ (d) $n = 2, \ell = 1, m = \pm 1$

19. A rigid rotator is in a quantum state described by the wavefunction

$$\psi(\theta,\varphi) = \sqrt{\frac{3}{4\pi}}\sin\theta\sin\varphi$$ **[TIFR 2014]**

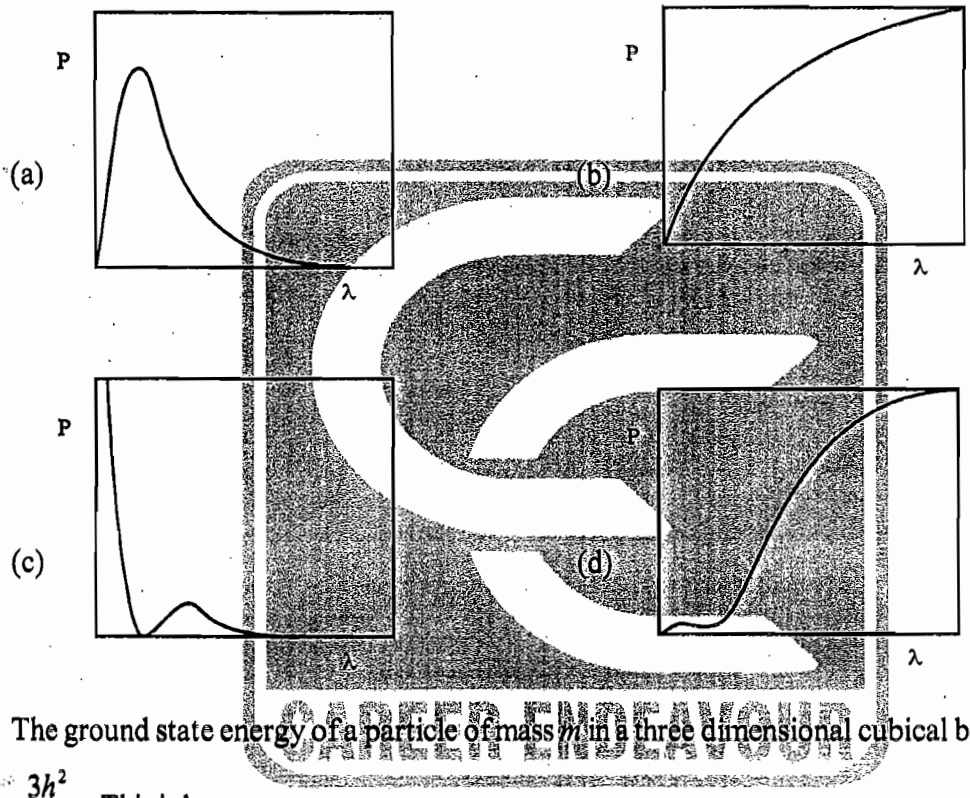
where θ and φ are the usual polar angles. If two successive measurements of L_z are made on this rotator, the probability that the second measurement will yield the value $+\hbar$ is

(a) 0.25 (b) 0.33 (c) 0.5 (d) negligible

20. A particle in the 2s state of hydrogen has the wave function

$$\psi_{2s}(r) = \frac{1}{4\sqrt{2}\,\pi}\left(\frac{1}{a_0}\right)^{3/2}\left(2-\frac{r}{a_0}\right)\exp\left(-\frac{r}{2a_0}\right)$$

where 'r' is the radial coordinate w.r.t. the nucleus as origin and a_0 is the Bohr radius. The probability P of finding the electron somewhere inside a sphere of radius λa_0 centred at the nucleus, is best described by the graph **[TIFR 2014]**



21. The ground state energy of a particle of mass m in a three dimensional cubical box of side ℓ is not zero but $\frac{3\hbar^2}{8m\ell^2}$. This is because **[TIFR 2015]**

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(a) The ground state has no nodes in the interior of the box.
(b) This is the most convenient choice of the zero level of potential energy.
(c) Position and momentum cannot be exactly determined simultaneously.
(d) The potential at the boundaries is not really infinite, but just very large.

22. Consider a particle of mass 'm' moving inside a two-dimensional square box whose sides are described by the equations $x = 0$, $x = L$, $y = 0$, $y = L$. What is the lowest eigenvalue of an eigenstate which changes sign under the exchange of x and y? **[JEST 2012]**

(a) $\frac{\hbar^2}{mL^2}$ (b) $\frac{3\hbar^2}{2mL^2}$ (c) $\frac{5\hbar^2}{2mL^2}$ (d) $\frac{7\hbar^2}{2mL^2}$

23. The binding energy of the hydrogen atom (electron bound to proton) is 13.6 eV. The binding energy of positronium (electron bound to positron) is **[JEST 2012]**

(a) 13.6/2 eV (b) 13.6/180 eV (c) 13.6×1810 eV (d) 13.6×2 eV

24. If a proton were ten times lighter, then the ground state energy of the electron in a hydrogen atom would have been **[JEST 2013, 2014]**

(a) Less (b) More (c) The same (d) Depends on the electron mass

25. Consider a quantum particle of mass 'm' in a three-dimensional isotropic simple harmonic potential $V(x,y,z)=\frac{1}{2}m\omega^2\left(x^2+y^2+z^2\right)$. It is known that the particle is in an energy eigenstate with eigenvalue $E=7\hbar\omega/2$. Which of the following cannot be the wave function of the particle? (In the following $\alpha=\sqrt{m\omega/\hbar}$ and $H_n(\xi)$ is the nth Hermite polynomial) **[JNU 2010]**

(a) $H_2(\alpha x)\exp\left(-\alpha\left(y^2+z^2\right)\right)$ (b) $H_2(\alpha x)\exp\left(-\alpha\left(x^2+y^2+z^2\right)\right)$

(c) $H_1(\alpha y)H_1(\alpha z)\exp\left(-\alpha\left(x^2+y^2+z^2\right)\right)$ (d) $H_1(\alpha x)H_1(\alpha z)\exp\left(-\alpha\left(x^2+y^2+z^2\right)\right)$

26. A particle of mass m is moving in a three-dimensional potential

$$V(x,y,z)=\frac{1}{2}m\omega^2\left(x^2+2y^2+4z^2\right)$$ **[JNU 2012]**

The energy of the particle in the ground state (lowest energy quantum state) is

(a) $\frac{\sqrt{7}}{2}\hbar\omega$ (b) $\frac{3}{2}\hbar\omega$ (c) $\frac{7}{2}\hbar\omega$ (d) $\frac{\left(3+\sqrt{2}\right)}{2}\hbar\omega$

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Chapter 6

Identical Particles

6.1 Introduction :

Identical Particles:

Particle having same intrinsic properties (mass, charge, spin) as known as identical particles.

There are two types of identical particles i.e.

(i) Classical identical particles (distinguishable)

Example:

Volume available for a gas molecule at NTP is $\sim 10^{-25}\,m^3$ and volume of single gas molecule $\sim 10^{-30}\,m^3$

So, we can identify every molecule of the gas. Hence, gas molecules are distinguishable.

(ii) Quantum identical particles (indistinguishable)

Example:

Volume available for each electron taking part in conduction within the metals is $\sim 10^{-28}\,m^3$ but the volume o a single electron is $\sim 10^{-27}\,m^3$. This shows that the electron wave functions overlap considerably and henc cannot be identified separately, i.e. they are indistinguishable.

- For a system of 'n' indistinguishable particles say electrons, we may be able to specify their positions, but it is not possible to say which electron is at a particular position. Therfore, interchanging the coordinates of any two electrons does not change the Hamiltonian. In other words, the Hamiltonian of the system is symmetric in coordinates of the particles i.e.,

$$\hat{H}(x_1, x_2, x_3 \ldots x_i, x_{i+1} \ldots x_n) = \hat{H}(x_1, x_2, x_3 \ldots x_{i+1}, x_i, \ldots x_n)$$

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Particle exchange operator:

This operator exchanges the particle in pair (both position and spin co-ordinates).

Example: Consider a system of 3 spinless particles and corresponding wave function at t =0 can be written as $\psi(\vec{r}_1, \vec{r}_2, \vec{r}_3)$. Then

$$\hat{P}_{12}\psi(\vec{r}_1, \vec{r}_2, \vec{r}_3) = \psi(\vec{r}_2, \vec{r}_1, \vec{r}_3)$$

$$\left(\hat{P}_{12}\right)^2 \psi(\vec{r}_1, \vec{r}_2, \vec{r}_3) = \psi(\vec{r}_1, \vec{r}_2, \vec{r}_3) \Rightarrow \quad \lambda^2 = 1 \Rightarrow \lambda = \pm 1$$

For $\lambda = 1$, $\hat{P}_{12}\psi(\vec{r}_1, \vec{r}_2, \vec{r}_3) = \psi(\vec{r}_1, \vec{r}_2, \vec{r}_3) = \psi(\vec{r}_2, \vec{r}_1, \vec{r}_3)$ i.e. the wave function $\psi(\vec{r}_1, \vec{r}_2, \vec{r}_3)$ is sym metric w.r.t exchange of particle 1 and particle 2.

For $\lambda = -1$, $\hat{P}_{12}\psi(\vec{r}_1, \vec{r}_2, \vec{r}_3) = -\psi(\vec{r}_1, \vec{r}_2, \vec{r}_3) = \psi(\vec{r}_2, \vec{r}_1, \vec{r}_3)$ i.e. the wave function $\psi(\vec{r}_1, \vec{r}_2, \vec{r}_3)$ is anti-symmetric w.r.t exchange of particle 1 and particle 2.

Note:

(i) Particle exchange operator is a hermi

(ii) Since particles are indistinguishable, any operator representing a physical property of the system must be symmetric w.r.t the particle exchange. Therefore, any operator representing a physical property commute with the particle exchange operator.

Symmetric wave function:

A wave function is said to be symmetric if interchange of any pair of particles leaves the wave function unchanged.

$$\psi_s(1,2,.....i,\ j....N) = \psi_s(1,2.....j,i,.....N)$$

The particles having symmetric wave function obey BE statistics and known as bosons.

Example: Photons (spin 1), neutral helium (spin 0), α-particle (spin 0), deutron (spin 1)

Anti-symmetric wave function:

A wave function is said to be anti-symmetric if interchange of any pair of particle changes the sign of the wave function.

$$\psi_a(1,2,.....i,j,.....N) = -\psi_a(1,2,.....j,i.....N)$$

The particles having anti-symmetric wave functions are known as fermions and follow FD statistics.

Example: Electron, protons, neutrons, muons (spin 1/2), Ω-particle (spin 3/2)

6.2 Symmetrization Postulate :

The state of the system containing N identical particles are either totally symmetric or totally anti symmetric under the exchange of any pair of particles and the states with mixed symmetry do not exist.

Note:

(i) Bosons have symmetric wave functions and Fermions have anti-symmetric wave functions

(ii) Wave function of a system of identical bosons is totally symmetric and of a system of identical fermions is totally anti-symmetric.

The total wave function corresponding to a system containing of N identical particles consisting of two parts (a) space part and (b) spin part, i.e.

Therefore, $\psi_{total} = \psi_{space} \times \chi_{spin}$

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(i) Both space part and spin part of total wave function of a system of identical bosons will be either symmetric or anti-symmetric.

$$\psi_{s,fermion} = \begin{cases} \psi_s(space) \times \chi_a(spin) \\ \psi_a(space) \times \chi_s(spin) \end{cases}$$

(ii) any one of the space part and spin part of total wave function of a system of identical fermions will be symmetric and other one is anti-symmetric.

$$\psi_{s,fermion} = \begin{cases} \psi_s(space) \times \chi_a(spin) \\ \psi_a(space) \times \chi_s(spin) \end{cases}$$

Composite Particles:

Consider a system of identical composite particles where each particle is composed of two or more identical particles. Spin of each composite particles can be obtained by adding the spin of its constituents. If total spin of the composite particles is half-integer, then the particle will behave as a fermion.

... then the particle will behave as a boson.

Example:

(i) A system of N identical H atoms. Each H atom consists of 1 proton and 1 electron (spin 1/2 each). Therefore, each H atom has spin 1 and it will behave as a boson. So, the system of N identical H atoms will have symmetric wave function.

(ii) ^4He (two protons and two neutrons) has integer spin and will behave as boson.

(iii) ^3He (two protons and one neutrons) has half integer spin and will behave as fermion.

6.3 Symmetric & anti-symmetric wave function (space part) :

For a system of 'n' non-interacting distinguishable particles, the wave function can be written as

$$\psi(\vec{r}_1,\vec{r}_2,\vec{r}_3.....\vec{r}_n) = \psi_1(\vec{r}_1).\psi_2(\vec{r}_2).\psi_3(\vec{r}_3).....\psi_n(\vec{r}_n)$$

But, for a system of 'n' non-interacting indistinguishable particles, the wave function will be different.

Example:

Consider a system of 2 non-interacting indistinguishable particles, in which one particle is in state 1 and the other particle is in state 2. Since, the particles are distinguishable, therefore the possible eigenfunctions are $\psi_1(\vec{r}_1)\psi_2(\vec{r}_2)$ and $\psi_1(\vec{r}_2)\psi_2(\vec{r}_1)$ and both are equal probable. The symmetric and anti-symmetric combinations for the wave function of the system of 2 particles will be

$$\psi_s(\vec{r}_1,\vec{r}_2) = \frac{1}{\sqrt{2}}\left[\psi_1(\vec{r}_1)\psi_2(\vec{r}_2) + \psi_1(\vec{r}_2)\psi_2(\vec{r}_1)\right]$$

$$\psi_a(\vec{r}_1,\vec{r}_2) = \frac{1}{\sqrt{2}}\left[\psi_1(\vec{r}_1)\psi_2(\vec{r}_2) - \psi_1(\vec{r}_2)\psi_2(\vec{r}_1)\right]$$

If both the particles are in the same state, then $\psi_a(\vec{r}_1,\vec{r}_2) = 0$ i.e. two identical fermions cannot occupy the same state. This is known as 'Pauli's exclusion principle'.

In general, if we take a system of N identical non-interacting indistinguishable particles and each particle is in a different state, then there will be $N!$ different type possible eiegenfunctions having same value of energy. The degenaracy arises due to the exchange of indistingushable particles and known as exchange degenaracy. The symmetric and anti-symmetric combinations for the wave function of the system of N particles will be

$$\psi_s(\vec{r}_1,\vec{r}_2,.....\vec{r}_N) = \frac{1}{\sqrt{N!}}\sum P\left[\psi_1(\vec{r}_1)\psi_2(\vec{r}_2)\psi_3(\vec{r}_3).....\psi_n(\vec{r}_N)\right]$$

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$$\psi_a(\vec{r}_1,\vec{r}_2,.....\vec{r}_N) = \frac{1}{\sqrt{N!}}\begin{vmatrix} \psi_1(\vec{r}_1) & \psi_1(\vec{r}_2) & ..... & \psi_1(\vec{r}_N) \\ \psi_2(\vec{r}_1) & \psi_2(\vec{r}_2) & ..... & \psi_2(\vec{r}_N) \\ \vdots & & & \\ \psi_N(\vec{r}_1) & \psi_N(\vec{r}_2) & ..... & \psi_N(\vec{r}_N) \end{vmatrix}$$

Note:

(i) If all the particles are in the same state i.e. $n_1 = n_2 = n_3 = ... = n_N$

$$\psi_s(\vec{r}_1,\vec{r}_2,\vec{r}_3,.....\vec{r}_N) = \prod_{i=1}^{N}\psi_n(\vec{r}_1)\psi_n(\vec{r}).....\psi_n(\vec{r}_N)$$

$$\psi_a(\vec{r}_1,\vec{r}_2,.....\vec{r}_N) = 0$$

(ii) If n_1 occurs N_1 times, n_2 occurs N_2 times, n_3 occurs N_3 times and so on .....

$$\psi_s(\vec{r}_1, \vec{r}_2, \vec{r}_3, ...\vec{r}_n) = \sqrt{\frac{N_1!\,N_2!\,N_3!.....N_N!}{N!}} \sum_P \hat{P}\psi_1(\vec{r}_1)\psi_2(\vec{r}_2).....\psi_n(\vec{r}_N)$$

6.4 Symmetric & anti-symmetric wave function (spin part) :

Spin functions for two-electron system:

Two electrons each having spin 1/2 i.e. $s_1 = \frac{1}{2}, s_2 = \frac{1}{2}$, then the total spin of two electrons will be

$$s = |s_1 + s_2|.....|s_1 - s_2| = 1, 0$$

and corresponding magnetic spin quantum number will be $m_s = 1, 0, -1, 0$

Therefore, the possible spin states will be $|s, m_s\rangle \equiv |0,0\rangle, |1,1\rangle, |1, 0\rangle, |1, -1\rangle$ and given as follows:

Symmetric Triplet state:

$$|1,1\rangle = |\uparrow\uparrow\rangle = |\alpha\alpha\rangle = \left|\frac{1}{2}, \frac{1}{2}\right\rangle \left|\frac{1}{2}, \frac{1}{2}\right\rangle$$

$$|1,-1\rangle = |\downarrow\downarrow\rangle = |\beta\beta\rangle = \left|\frac{1}{2}, -\frac{1}{2}\right\rangle \left|\frac{1}{2}, -\frac{1}{2}\right\rangle$$

$$|1,0\rangle = \frac{1}{\sqrt{2}}\left[|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right] = \frac{1}{\sqrt{2}}\left[|\alpha\beta\rangle + |\beta\alpha\rangle\right]$$

$$= \frac{1}{\sqrt{2}}\left[\left|\frac{1}{2}, \frac{1}{2}\right\rangle \left|\frac{1}{2}, -\frac{1}{2}\right\rangle + \left|\frac{1}{2}, -\frac{1}{2}\right\rangle \left|\frac{1}{2}, \frac{1}{2}\right\rangle\right]$$

Anti-symmetric Singlet state:

$$|0,0\rangle = \frac{1}{\sqrt{2}}\left[|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right] = \frac{1}{\sqrt{2}}\left[|\alpha\beta\rangle - |\beta\alpha\rangle\right]$$

$$= \frac{1}{\sqrt{2}}\left[\left|\frac{1}{2}, \frac{1}{2}\right\rangle \left|\frac{1}{2}, -\frac{1}{2}\right\rangle - \left|\frac{1}{2}, -\frac{1}{2}\right\rangle \left|\frac{1}{2}, \frac{1}{2}\right\rangle\right]$$

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For a system of N identical non-interacting indistinguishable particles each having spin 's', total number of possible spin states is $(2s+1)^N$.

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Example 1. N non interacting bosons are in an infinite potential well defined by $V(x) = 0$ for $0 < x < a$; $V(x) = \infty$ for $x < 0$ and for $x > a$. Find the ground state energy of the system. What would be the ground state energy if the particles are fermions.

Soln. The energy eigenvalue of a particle in the infinite square well is given by

$$E_n = \frac{\pi^2\hbar^2 n^2}{2ma^2}, \qquad n = 1, 2, 3, ...$$

As the particles are bosons, all the N particles will be in the $n = 1$ state in the ground state configuration. Hence, the ground state energy of the configuration will be

$$E = \frac{N\pi^2\hbar^2}{2ma^2}$$

If the particles are fermions, a state can have only two of them, one spin up and the other spin down

Therefore, the lowest N/2 states will be filled. The total ground state energy will be

$$E = 2\frac{\pi^2\hbar^2}{2ma^2}[1^2 + 2^2 + 3^3 + ... + (N/2)^2]$$

$$= \frac{\pi^2\hbar^2}{ma^2}\frac{1}{6}\left[\frac{N}{2}\left(\frac{N}{2}+1\right)\left(2\frac{N}{2}+1\right)\right]$$

$$= \frac{\pi^2\hbar^2}{24ma^2}N(N+1)(N+2)$$

Example 2. Consider two noninteracting electrons described by the Hamiltonian

$$H = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + V(x_1) + V(x_2)$$

where $V(x) = 0$ for $0 < x < a$; $V(x) = \infty$ for $x < 0$ and for $x > a$. If both the electrons are in the same spin state, what is the lowest energy and eigenfunction of the two-electron system?

Soln. As both the electrons are in the same spin state, the possible combinations of spin part of the wave functions will be $|\uparrow\uparrow\rangle$ or $|\downarrow\downarrow\rangle$, both being symmetric. Since, the system contains two electrons (fermions), then the total wave function of the sytem will be anti-symmetric. Hence the space function must be antisymmetric. Therefore, both electrons cannot be in the same state. So, ground state energy will corresponds to $n_1 = 1, n_2 = 2$

Ground state energy $(n_1 = 1, n_2 = 2) = \frac{\pi^2\hbar^2}{2ma^2} + \frac{4\pi^2\hbar^2}{2ma^2} = \frac{5\pi^2\hbar^2}{2ma^2}$

Since, the electrons are indistinguishable, therefore the antisymmetric combination for the space part is

$$\frac{1}{\sqrt{2}}[\psi_1(\vec{r}_1)\psi_2(\vec{r}_2) - \psi_1(\vec{r}_2)\psi_2(\vec{r}_1)]$$

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Example 3. Sixteen noninteracting electrons are confined in a potential

$$V(x) = \infty \text{ for } x < 0 \text{ and } x > 0;\ V(x) = 0, \text{ for } 0 < x < a.$$

(i) What is the energy of the least energetic electron in the ground state?

(ii) What is the energy of the most energetic electron in the ground state?

(iii) What is the Fermi energy E_f of the system?

Soln. (i) The least energetic electron in the ground state is given by $E_1 = \frac{\pi^2\hbar^2}{2ma^2}$.

(ii) In the given potential, the energy eigenvalue

$$E_n = \frac{\pi^2\hbar^2 n^2}{2ma^2}, \qquad n = 1, 2, 3, ...$$

As two electrons can go into each of the states $n = 1, 2, 3, ...$, the highest filled level will have n=8 and its energy will be

$$E_8 = \frac{\pi^2\hbar^2 8^2}{2ma^2} = \frac{32\pi^2\hbar^2}{ma^2}$$

(iii) The energy of the highest filled state is the Fermi energy E_F. Hence,

$$E_F = \frac{32\pi^2\hbar^2}{ma^2}$$

Example 4. What is the ground state energy and wave function for two identical particles in the potential defined in problem if the two particles are (i) bosons, and (ii) fermions?

Soln. (i) Bosons: Both the particles can be in the same state. Hence, ground state will correspond to $n_1 = 1, n_2 = 1$ and the corresponding space part will be symmetric in nature.

The energy and wave function of the combined system are

$$E = E_1(1) + E_1(2) = \frac{\pi^2\hbar^2}{ma^2}, \quad \psi = \psi_1(x_1)\psi_2(x_2) = \left(\frac{2}{a}\right)\sin\frac{\pi x_1}{a}\sin\frac{\pi x_2}{a}$$

The spin part of the wave function of the two particle system must be symmetric.

The wave function of the two particle system including spin is

$$\psi(space)\chi_s(spin) = \left(\frac{2}{a}\right)\sin\frac{\pi x_1}{a}\sin\frac{\pi x_2}{a}\begin{cases}\alpha\alpha\\ \beta\beta\\ (\alpha\beta+\beta\alpha)/\sqrt{2}\end{cases}$$

(ii) Fermions: In the ground state, one particle has to be spin up and the other spin down. Therefore, the spin part of the wave function will be anti-symmetric in nature. Hence the energy and wave functions are

$$E = \frac{\pi^2\hbar^2}{ma^2}, \quad \psi(space)\chi_s(spin) = \left(\frac{2}{a}\right)\sin\frac{\pi x_1}{a}\sin\frac{\pi x_2}{a}\left[\frac{1}{\sqrt{2}}(\alpha\beta-\beta\alpha)\right]$$

Example 5. Consider a system of two identical particles occupying any of three energy levels A, B and C having energies E, $2E$ and $3E$, respectively. The level A is doubly degenerate (A_1 and A_2) and the system is in thermal equilibrium. Find the possible configurations and the corresponding energy in the following cases:

(i) the particles obey Fermi statistics;

(ii) the particles obey Bose statistics; and

(iii) the particles are distinguishable and obey Boltzmann statistics.

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Soln. Denote the two states with energy E by A_1 and A_2, and the states with 2E and 3E by B and C, respectively. If particle 1 is in A_1 and particle 2 is in A_2, the configuration is marked as (A_1, A_2). Thus, the symbol (B, C) indicates that one particle is in B and the other is in C.

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(i) If the particles obey Fermi statistics, the system has the following configuration and energy.

Configuration:	(A_1, A_2),	(A_1, B),	(A_2, B),	(A_1, C),	(A_2, C),	(B, C)
Energy:	2E	3E	3E	4E	4E	5E

(ii) If the particles obey Bose statistics, the additional configuration: (A_1, A_1), (A_2, A_2), (B, B) and (C, C) are also possible. Hence the configuration and energy are

(A_1, A_2),	(A_1, B),	(A_2, B),	(A_1, C),	(A_2, C),	(B, C),	(A_1, A_1),	(A_2, A_2),	(B, B),	(C, C),
2E,	3E,	3E,	4E,	4E,	5E,	2E,	2E,	4E,	6E

(iii) Since the particles are distinguishable, the following configurations are also possible:

Configuration:	(A_2, A_1),	(B, A_1),	(B, A_2),	(C, A_1),	(C, A_2),	(C, B)
Energy:	2E,	3E,	3E,	4E,	4E,	5E

Example 6. A one-dimensional potential well has the single-particle energy eigenfunctions $\psi_1(x)$ and $\psi_2(x)$ corresponding to energies E_1 and E_2 for the two lowest states. Two noninteracting particles are placed in the well. Obtain the two lowest total energies of the two particle system with the wavefunction and degeneracy if the particles are (i) distinguishable spin-half particles, (ii) identical spin half particles, and (iii) identical spin zero particles.

Soln. (i) Distinguishable spin-half particles. The particles have spin = half. Hence the total spin $S = 0$, 1 when $S = 0$, $M_s = 0$ and when $S = 1$, $M_s = 1, 0, -1$. Let us denote the spin wave functions by the corresponding $|SM_s\rangle$. As the particles are distinguishable, the two particles can be in ψ_1 even when $S = 1$. The different wave functions and energies are

$$\psi_1(x_1)\psi_1(x_2)|00\rangle, \qquad E_1 + E_1 = 2E_1$$

$$\psi_1(x_1)\psi_1(x_2)|1M_s\rangle, \qquad M_s = 1, 0, -1, \qquad E_1 + E_1 = 2E_1$$

The degeneracy is 1 + 3 = 4

(ii) Two identical spin-half particles. Again, the total spin $S = 0$ or 1. When $S = 0$, the two particles are in ψ_1 with their spins in the opposite directions. The total wave function must be antisymmetric. The space part of the wave function is symmetric. Hence the spin part must be antisymmetric. The wave function of the system is

$$\psi_1(x_1)\psi_1(x_2)\frac{1}{\sqrt{2}}[\alpha(1)\beta(2) - \beta(1)\alpha(2)]$$

with energy $E_1 + E_1 = 2E_1$.

When $S = 1$, one particle will be in level 1 and the other will be in level 2. Hence, the symmetric and antisymmetric combinations of space functions are

$$\psi_s = \frac{1}{\sqrt{2}}[\psi_1(x_1)\psi_2(x_2) + \psi_1(x_2)\psi_2(x_1)]$$

Example 7. A system of 2 identical bosons, each of mass 'm' is placed in a 1-D box of length 'L'. Both particles are in same spin state. The energy of the system is $\frac{5\pi^2\hbar^2}{2mL^2}$. What is the space part of the wave function?

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Soln. $E = \frac{\pi^2\hbar^2}{2mL^2}\left(n_1^2 + n_2^2\right) = \frac{5\pi^2\hbar^2}{2mL^2} \Rightarrow n_1 = 1$ or $n_1 = 2 \Rightarrow n_2 = 2 \quad n_2 = 1$

Since, $\psi_t = \psi_{space} \times \psi_{spin}$

where, ψ_{space} = symmetric and ψ_{spin} = symmetric as two bosons are of same spin.

Therefore, the symmetric part of the wave function will be

$$\psi_{space} = \frac{1}{\sqrt{2}}\left[\psi(1,2) + \psi(2,1)\right]$$

$$= \frac{1}{\sqrt{2}}\left(\frac{2}{L}\right)\left[\sin\frac{\pi x_1}{L}\sin\frac{2\pi x_2}{L} + \frac{\sin 2\pi x_1}{L}\sin\frac{\pi x_2}{L}\right]$$

Example 8. Consider a wave function $\psi = \psi(\vec{r}_1, \vec{r}_2)\chi_s$ for a fermionic system consisting of two spin ½ particles. The spatial part of the wave function is given by

$$\psi(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}}\left[\phi_1(\vec{r}_1)\phi_2(\vec{r}_2) + \phi_1(\vec{r}_2)\phi_1(\vec{r}_1)\right]$$

The spin part of the wave function will be

(a) $\frac{1}{\sqrt{2}}(\alpha\beta + \beta\alpha)$ (b) $\frac{1}{\sqrt{2}}(\alpha\beta - \beta\alpha)$ (c) $(\alpha\alpha)$ (d) $(\beta\beta)$

Soln. Given space part of the wave function is symmetric nature and $\psi_{total} = \psi_{space} \times \psi_{spin}$ = antisymmetric ,

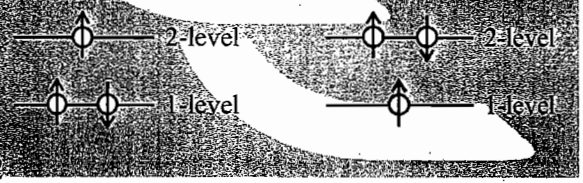
therefore spin part of the wave function will anti-symmetric i.e. $\chi_{spin} = \frac{1}{\sqrt{2}}(\alpha\beta - \beta a)$

Correct answer is (b)

CSIR PREVIOUS YEAR QUESTIONS

1. Three identical spin-1/2 fermions are to be distributed in two non-degenerate distinct energy levels. The number of ways this can be done is **[CSIR Dec 2013]**
(a) 8 (b) 4 (c) 3 (d) 2

Soln. The maximum number of particles with spin's can be filled in a non-degenerate energy level = 2s + 1.
Fermians are quantum particles and quantum identical particles are in general indistinguishable. If we include the concept of indistinguishability then three identical spin-½ particles (fermians) can be distributed in two non-degenerate distinct energy levels as



The number of ways = 2

On changing the direction of spin or orientation of spin, all the distribution will be identical. If we include the concept of distinguishability due to spin or we distinguish the particles due to spin the 3-identical particles with spin-½ can be distributed in two non-degenerate energy levels as

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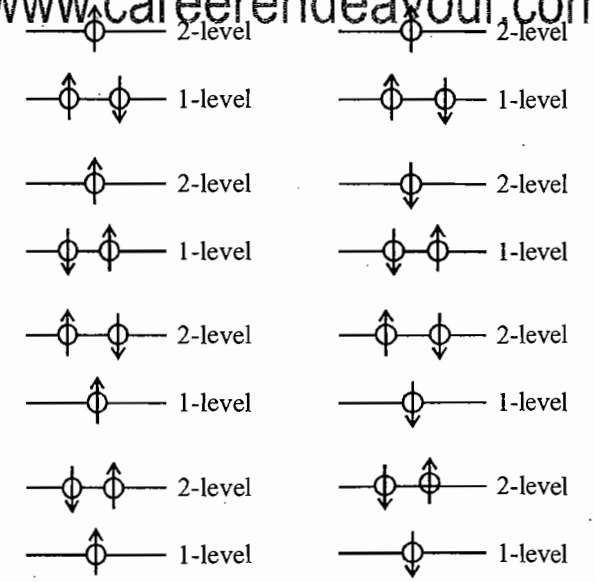

The number of ways = 8

But quantum identical particles are in general indistinguishable and there is no hint to consider particles distinguishable.

Correct answer is (d)

2. Consider a system of two non-interacting identical fermions, each of mass m in an infinite square well potential of width a. (Take the potential inside the well to be zero and ignore spin). The composite wavefunction for the system with total energy

$$E = \frac{5\pi^2\hbar^2}{2ma^2}$$

is **[CSIR June 2014]**

(a) $\frac{2}{a}\left[\sin\left(\frac{\pi x_1}{a}\right)\sin\left(\frac{2\pi x_2}{a}\right) - \sin\left(\frac{2\pi x_1}{a}\right)\sin\left(\frac{\pi x_2}{a}\right)\right]$

(b) $\frac{2}{a}\left[\sin\left(\frac{\pi x_1}{a}\right)\sin\left(\frac{2\pi x_2}{a}\right) + \sin\left(\frac{2\pi x_1}{a}\right)\sin\left(\frac{\pi x_2}{a}\right)\right]$

(c) $\frac{2}{a}\left[\sin\left(\frac{\pi x_1}{a}\right)\sin\left(\frac{3\pi x_2}{2a}\right) - \sin\left(\frac{3\pi x_1}{2a}\right)\sin\left(\frac{\pi x_2}{a}\right)\right]$

(d)

Soln. A system of two non-interacting identical fermions have anti-symmetric wave function.

If we ignore the spin of the fermions, then space part of the wave function will be anti-symmetric.

Energy of the system $= \frac{\pi^2\hbar^2}{2ma^2}\left(n_1^2 + n_2^2\right)$

Given : $\frac{\pi^2\hbar^2}{2ma^2}\left(n_1^2 + n_2^2\right) = \frac{5\pi^2\hbar^2}{2ma^2} \Rightarrow n_1 = 1, n_2 = 2$

The space part wavefunction of the system

$$= \frac{1}{\sqrt{2}}\left[\psi_{n_1}(x_1)\psi_{n_2}(x_2) + \psi_{n_2}(x_1)\psi_{n_1}(x_2)\right]$$

$$= \frac{1}{\sqrt{2}}\left[\frac{2}{a}\sin\left(\frac{\pi x_1}{a}\right)\sin\left(\frac{2\pi x_2}{a}\right) - \frac{2}{a}\sin\left(\frac{2\pi x_1}{a}\right)\sin\left(\frac{\pi x_2}{a}\right)\right]$$

Correct answer is (a)

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PRACTICE SET

1. Consider the wavefunction $\psi = \psi(\vec{r}_1, \vec{r}_2)\chi_s$ for a fermionic system consisting of two spin-half particles. The spatial part of the wavefunction is given by **[GATE 2012]**

$$\psi(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}}\left[\phi_1(\vec{r}_2)\phi_2(\vec{r}_2) + \phi_2(\vec{r}_1)\phi_1(\vec{r}_2)\right]$$

Where ϕ_1 and ϕ_2 are single particle states. The spin part χ_s of the wavefunction with spin states $\alpha\left(+\frac{1}{2}\right)$ and $\beta\left(-\frac{1}{2}\right)$ should be

(a) $\frac{1}{\sqrt{2}}(\alpha\beta + \beta\alpha)$ (b) $\frac{1}{\sqrt{2}}(\alpha\beta - \beta\alpha)$ (c) $\alpha\alpha$ (d) $\beta\beta$

2. The ground state and the first excited state wave functions of a one dimensional infinite potential well are ψ_1 and ψ_2, respectively. When two spin-up electrons are placed in this potential, which one of the following, with x_1 and x_2 denoting the position of the two electrons, correctly represents the space part of the ground state wave function of the system? **[GATE 2014]**

(a) $\frac{1}{\sqrt{2}}\left[\psi_1(x_1)\psi_2(x_1) - \psi_1(x_2)\psi_2(x_2)\right]$ (b) $\frac{1}{\sqrt{2}}\left[\psi_1(x_1)\psi_2(x_2) + \psi_1(x_2)\psi_2(x_1)\right]$

(c) $\frac{1}{\sqrt{2}}\left[\psi_1(x_1)\psi_2(x_1) + \psi_1(x_2)\psi_2(x_2)\right]$ (d) $\frac{1}{\sqrt{2}}\left[\psi_1(x_1)\psi_2(x_2) - \psi_1(x_2)\psi_2(x_1)\right]$

3. Which one of the following is a fermion? **[GATE 2014]**

(a) α – particle (b) ${}_4Be^7$ nucleus (c) Hydrogen atom (d) Deuteron

4. The spatial part of a two-electron state is symmetric under exchange. If $|\uparrow\rangle$ and $|\downarrow\rangle$ represent the spin-up and spin-down states respectively of each particle, the spin-part of the two-particle state is **[JEST 2012]**

(a) $|\uparrow\rangle|\uparrow\rangle$ (b) $|\uparrow\rangle|\downarrow\rangle$

(c) $\left(|\downarrow\rangle|\uparrow\rangle - |\uparrow\rangle|\downarrow\rangle\right)/\sqrt{2}$ (d) $\left(|\downarrow\rangle|\uparrow\rangle + |\uparrow\rangle|\downarrow\rangle\right)/\sqrt{2}$

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5. Two electrons are confined in a one dimensional box of length L. The one-electron states are given by $\psi_n(x) = \sqrt{2/L}\sin(n\pi x/L)$. What would be the ground state wave function $\psi(x_1, x_2)$ if both electrons are arranged to have the same spin state? **[JEST 2013]**

(a) $\psi(x_1, x_2) = \frac{1}{\sqrt{2}}\left[\frac{2}{L}\sin\left(\frac{\pi x_1}{L}\right)\sin\left(\frac{2\pi x_2}{L}\right) + \frac{2}{L}\sin\left(\frac{2\pi x_1}{L}\right)\sin\left(\frac{\pi x_2}{L}\right)\right]$

(b) $\psi(x_1, x_2) = \frac{1}{\sqrt{2}}\left[\frac{2}{L}\sin\left(\frac{\pi x_1}{L}\right)\sin\left(\frac{2\pi x_2}{L}\right) - \frac{2}{L}\sin\left(\frac{2\pi x_1}{L}\right)\sin\left(\frac{\pi . x_2}{L}\right)\right]$

(c) $\psi(x_1, x_2) = \frac{2}{L}\sin\left(\frac{\pi x_1}{L}\right)\sin\left(\frac{2\pi x_2}{L}\right)$

(d) $\frac{2}{L}\sin\left(\frac{2\pi x_1}{L}\right)\sin\left(\frac{\pi x_2}{L}\right)$

Chapter 7

Perturbation Theory

7.1. Time Independent perturbation theory :

The potential energy of most of the real systems are different from the standard potentials that have been considered till now, and an exact solution is not possible. Different approximate methods have been devoloped to obtain the approximate solutions of those systems. One such method is time-independent perturbation.

Non-degenerate Perturbation Theory

In the time independent perturbation approach, the Hamiltonian of the system can be written as

$$\hat{H} = \hat{H}_0 + \hat{H}'$$

where $\hat{H}_0$ is the unperturbed Hamiltonian, whose nondegenerate energy eigenvalues $E_n^0\ (n = 0,1,2.....)$ and corresponding eigenfunctions $\psi_n^0\ (n = 0,1,2.....)$ are assumed to be known. The functions $\psi_n^0\ (n = 0,1,2.....)$ form a complete orthonormal basis and $\hat{H}'$ is the time independent perturbing Hamiltonian.

First order correction to energy of the nth state $= E_n^{(1)} = \left\langle \psi_n^0 \middle| H' \middle| \psi_n^0 \right\rangle$

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First order correction to wave function of the nth state $= \psi_n^{(1)} = \sum_{m \neq n} \frac{\left\langle \psi_m^0 \middle| H' \middle| \psi_n^0 \right\rangle}{E_n^0 - E_m^0} \left| \psi_m^0 \right\rangle$

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Second order correction to energy of the nth state $= E_n^{(2)} = \sum_{m \neq n} \frac{\left| \left\langle \psi_m^0 \middle| H' \middle| \psi_n^0 \right\rangle \right|^2}{E_n^0 - E_m^0}$

Example 1: A particle of mass m_0 and charge 'e' oscillates along the the x-axis in a one-dimensional harmonic potential with an angular frequency ω. If an electric field ε is applied along the x-axis, evaluate the first and second order corrections to the energy of the nth state.

Soln. The potential energy due to the field $\varepsilon = -\vec{p}.\vec{E} = -e\varepsilon x$

The perturbation $H' = -e\varepsilon x = -e\varepsilon \sqrt{\frac{\hbar}{2m_0\omega}} \left(\hat{a} + \hat{a}^\dagger\right)$

First order correction to energy $= E_n^{(1)} = -e\varepsilon \sqrt{\frac{\hbar}{2m_0\omega}} \left\langle n \middle| \left(\hat{a} + \hat{a}^\dagger\right) \middle| n \right\rangle = 0$

Second order correction to energy $= E_n^{(2)} = \sum_{m \neq n} \frac{\left|\langle n|H'|m\rangle\right|^2}{E_n^0 - E_m^0}$

Now, $\langle n|H'|m\rangle = -e\varepsilon\sqrt{\frac{\hbar}{2m_0\omega}}\langle n|a + a^\dagger|m\rangle$

Here, m can take all integral values except n. The non-vanishing elements corresponds to $m = (n+1)$ and $(n-1)$. Hence,

Therefore, $E_n^{(2)} = e^2\varepsilon^2 \frac{\hbar}{2m_0\omega}\left[\frac{\left(\sqrt{n+1}\right)^2}{-\hbar\omega} + \frac{\left(\sqrt{n}\right)^2}{\hbar\omega}\right] = -\frac{e^2\varepsilon^2}{2m_0\omega^2}$

Example 2. Evaluate the first and second order correction to the energy of the n = 1 state of an oscillator of mass 'm' and angular frequency 'ω' subjected to a potential.

$$V(x) = \frac{1}{2}m\omega^2x^2 + bx, \qquad bx << \frac{1}{2}m\omega^2x^2$$

Soln. The first order correction to energy for the n = 1 state is given by

$$E_1^{(1)} = \langle 1|bx|1\rangle = b\sqrt{\frac{\hbar}{2m\omega}}\langle 1|\left(\hat{a} + \hat{a}^\dagger\right)|1\rangle = 0$$

Using, $a|n\rangle = \sqrt{n}\,|n-1\rangle$ and $a^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle$

The second order correction to energy for the n = 1 state is given by

$$E_1^{(2)} = b^2\left(\frac{\hbar}{2m\omega}\right)\sum_{k\neq 1}\frac{\left|\langle 1|\left(\hat{a} + \hat{a}^\dagger\right)|k\rangle\right|^2}{E_1^0 - E_k^0} = b^2\left(\frac{\hbar}{2m\omega}\right)\left[\frac{1}{E_1^0 - E_0^0} + \frac{2}{E_1^0 - E_2^0}\right]$$

$$= b^2\left(\frac{\hbar}{2m\omega}\right)\left(\frac{1}{\hbar\omega} - \frac{2}{\hbar\omega}\right) = -\frac{b^2}{2m\omega^2}$$

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Example 3. A one-dimensional box of length 'a' conatins two particles each of mass 'm'. The interactiuon between the particles is described by a potential of the type $V(x_1, x_2) = \lambda\delta(x_1 - x_2)$, which is the δ-Dirac delta function. Calculate the ground state energy to first order in λ.

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Soln. The interaction between the particles can be treated as the perturbation. The Hamiltonian without that will be the unperturbed part. Without the δ-potential.

$$V(x_1, x_2) = \begin{cases} 0, & 0 \le x_1, x_2 \le a \\ \infty, & \text{otherwise} \end{cases}$$

The unperturbed Hamiltonian is $H_0 = -\frac{\hbar^2}{2m}\frac{d^2}{dx_1^2} - \frac{\hbar^2}{2m}\frac{d^2}{dx_2^2} + V(x_1, x_2)$

From the results of an infinitely deep potential well, the energy and wave functions are

$$E_{n_xn_y} = \frac{\pi^2\hbar^2}{2ma^2}\left(n_x^2 + n_y^2\right), \qquad n_x, n_y = 1, 2, 3, \ldots\ldots$$

$$\psi_{n_x n_y}(x_1,x_2)=\psi_{n_x}(x_1)\psi_{n_y}(x_2)=\frac{2}{a}\sin\left(\frac{n_x\pi x_1}{a}\right)\sin\left(\frac{n_y\pi x_2}{a}\right)$$

For the ground state, $n_x=1, n_y=1$, we have

$$E_{11}^0=\frac{\pi^2\hbar^2}{ma^2},\quad \psi_{11}^0(x_1,x_2)=\frac{2}{a}\sin\left(\frac{\pi x_1}{a}\right)\sin\left(\frac{\pi x_2}{a}\right)$$

Perturbing Hamiltonian $H'=\lambda\delta(x_1-x_2)$

The first order correction to the ground state energy

$$\Delta E=\left\langle\psi_{11}^0\middle|H'\middle|\psi_{11}^0\right\rangle$$

$$=\left(\frac{2}{a}\right)^2\int_0^a\int_0^a\lambda\delta(x_1-x_2)\sin^2\left(\frac{\pi x_1}{a}\right)\sin^2\left(\frac{\pi x_2}{a}\right)dx_1dx_2$$

$$=\left(\frac{2}{a}\right)^2\lambda\int_0^a\sin^4\left(\frac{\pi x_1}{a}\right)dx_1=\frac{4\lambda}{a^2}\frac{3}{8}a=\frac{3\lambda}{2a}$$

Therefore, the ground state energy corrected upto first order is

$$E_{11}=E_{11}^0+\Delta E=\frac{\pi^2\hbar^2}{ma^2}+\frac{3\lambda}{2a}$$

Example 4. Consider the infinite square well defined by

$$V(x)=0 \text{ for } 0\le x<a$$

$$V(x)=\infty \text{ otherwise}$$

Using the first order perturbation theory, calculate the energy of the first two states of the potential well if a portion defined by $V(x)=V_0x/a$, where V_0 is a small constant, with $0\le x\le a$ being sliced off.

Soln. The energy eigenvalues and normalized eigenfunctions of the n^{th} state of unperturbed Hamiltonian are

$$E_n^0=\frac{n^2\pi^2\hbar^2}{2ma^2},\psi_n^0=\sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a},\quad n=1,2,3,....$$

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The perturbation $H'=V_0x/a$ which is depicted in figure below.

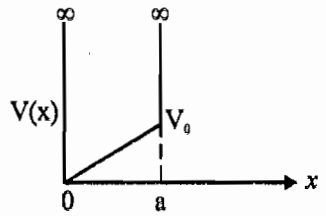

Figure: Sliced infinite potential well.

The first order correction to the energy for the n = 1 state is

$$E_1^{(1)}=\left\langle\psi_1^0\middle|\frac{V_0x}{a}\middle|\psi_1^0\right\rangle=\frac{V_0}{a}\frac{2}{a}\int_0^a x\sin^2\frac{\pi x}{a}dx$$

$$= \frac{2V_0}{a^2}\int_0^a \frac{x}{2}\left(1-\cos\frac{2\pi x}{a}\right)dx = \frac{2V_0}{a^2}\int_0^a \frac{x}{2}dx - \frac{2V_0}{a^2}\int_0^a \frac{x}{2}\cos\frac{2\pi x}{a}dx$$

$$= \frac{V_0}{2} + 0 = \frac{V_0}{2}$$

The first order correction to the enegry for the n = 2 state is

$$E_2^{(1)} = \left\langle \psi_2^0 \left| \frac{V_0 x}{a} \right| \psi_2^0 \right\rangle = \frac{V_0}{a}\frac{2}{a}\int x \sin^2\frac{2\pi x}{a}dx = \frac{V_0}{2}$$

The ground state and first excited energies corrected upto first order are

$$\frac{\pi^2\hbar^2}{2ma^2} + \frac{V_0}{2} \text{ and } \frac{2\pi^2\hbar^2}{ma^2} + \frac{V_0}{2}$$

Example 5. A particle of mass 'm' moves in an infinite one-dimensional box of bottom 'a' with a potential dip as defined by

$$V(x) = \infty \text{ for } x < 0 \text{ and } x > a$$

$$V(x) = -V_0 \text{ for } 0 < x < \frac{a}{3}$$

$$V(x) = 0 \text{ for } \frac{a}{3} < x < a$$

Find the first order energy of the ground state.

Soln. For a particle in the infinite potential well defined by $V(x) = 0$ for $0 < x < a$ and $V(x) = \infty$ otherwise, the energy eigenvalues and normalized eigenfunctions are

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}, \psi_n = \sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a}; \quad n = 1, 2, 3, \ldots$$

The perturbing Hamiltonian is $H' = -V_0$ for $0 < x < a/3$

The first order energy correction to the ground state is

$$E_0^{(1)} = -\frac{2}{a}V_0\int_0^{a/3}\sin^2\frac{\pi x}{a}dx$$

$$= -\frac{2}{a}V_0\int_0^{a/3}\frac{1}{2}\left(1-\cos\frac{2\pi x}{a}\right)dx$$

$$= -\frac{V_0}{a}[x]_0^{a/3} + \frac{V_0}{a}\frac{a}{2\pi}\left[\sin\frac{2\pi x}{a}\right]_0^{a/3}$$

$$= -\frac{V_0}{3} + \frac{V_0}{4\pi} \times 0.866 = -0.264\,V_0$$

The energy of the ground state corrected to first order is

$$E_1' = \frac{\pi^2\hbar^2}{2ma^2} - 0.264V_0$$

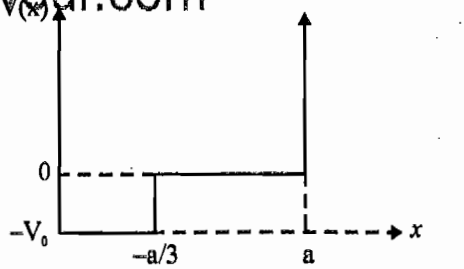

Figure: Infinite square well with potential dip

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Example 6. A rigid rotator in a plane is acted on by a perturbation represented by

$$H' = \frac{V_0}{2}\left(3\cos^2\phi - 1\right),\ V_0 = \text{constant}$$

Calculate the ground state up to the second orer in the perturbation.

Soln. The energy eigenvalues and normalized eigenfunctions of a plane rotator are given by

$$E_m = \frac{m^2\hbar^2}{2I}, \quad m = 0, \pm 1, \pm 2, ...$$

$$\psi_m(\phi) = \frac{1}{\sqrt{2\pi}}\exp(im\phi)$$

Except the ground state, all levels are doubly degenerate. The first order correction to the ground state energy is

$$E_0^{(1)} = \langle\psi_0|H'|\psi_0\rangle = \left\langle\psi_0\left|\frac{V_0}{2}\left(3\cos^2\phi - 1\right)\right|\psi_0\right\rangle = \left\langle\psi_0\left|\frac{3V_0}{2}\cos^2\phi\right|\psi_0\right\rangle - \left\langle\psi_0\left|\frac{V_0}{2}\right|\psi_0\right\rangle$$

$$= \frac{3}{4}V_0 - \frac{V_0}{2} = \frac{V_0}{4}$$

The second order energy correction to the ground state energy

$$E_0^{(2)} = \sum_{m\neq 0}\frac{\left|\langle\psi_0|H'|\psi_m\rangle\right|^2}{E_0^0 - E_m^0}$$

$$\langle\psi_0|H'|\psi_m\rangle = \frac{V_0}{2}\int_0^{2\pi}\frac{1}{\sqrt{2\pi}}\left(3\cos^2\phi - 1\right)\frac{1}{\sqrt{2\pi}}e^{im\phi}d\phi$$

$$= \frac{3V_0}{4\pi}\int_0^{2\pi}\cos^2\phi\, e^{im\phi} - \frac{V_0}{4\pi}\int_0^{2\pi}e^{im\phi}d\phi$$

$$= \frac{3V_0}{8\pi}\int_0^{2\pi}(1+\cos 2\phi)e^{im\phi}d\phi = \frac{3V_0}{8\pi}\int_0^{2\pi}\cos 2\phi\, e^{im\phi}d\phi$$

$$= \frac{3V_0}{16\pi}\int_0^{2\pi}\left(e^{i2\phi} + e^{-i2\phi}\right)e^{im\phi}d\phi$$

$$= \frac{3V_0}{16\pi}\int_0^{2\pi}e^{i(m+2)\phi}d\phi + \frac{3V_0}{16\pi}\int_0^{2\pi}e^{i(m-2)\phi}d\phi$$

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The first integral is finite when m = -2, the second integral is finite when m = +2 and their values are equal to $3V_0/8$. $E_{\pm 2} = 2\hbar^2/I, E_0 = 0$.

Hence, $E_0^0 - E_2^0 = E_0^0 - E_{-2}^0 = -\frac{2\hbar^2}{I}$

Therefore, the ground state energy corrected to second order

$$E_0^{(2)} = \frac{(3V_0/8)^2}{2\hbar^2/I} + \frac{(3V_0/8)^2}{2\hbar^2/I} = -\frac{9}{64}\frac{V_0^2 I}{\hbar^2}$$

Example 7. The matrices for the unperturbed (H^0) and perturbation (H') Hamiltonian in the orthonormal basis $|\phi_1\rangle$ and $|\phi_2\rangle$ are

$$H^0 = \begin{pmatrix} E_0 + \varepsilon & 0 \\ 0 & E_0 - \varepsilon \end{pmatrix}, \qquad H' = \begin{pmatrix} 0 & A \\ A & 0 \end{pmatrix}$$

Determine (i) the first order correction to energy, (ii) second order correction to energy, and (iii) the wave function corrected to first order.

Soln. (i) The first order correction to the energy is zero since the perturbation matrix has no diagonal element.

(ii) The energy correction upto second order is

$$E_1^{(2)} = \frac{|\langle 1|H'|2\rangle|^2}{E_1^0 - E_2^0} = \frac{|A|^2}{2\varepsilon} = \frac{A^2}{2\varepsilon}, \; E_2^{(2)} = \frac{|\langle 2|H'|1\rangle|^2}{E_2^0 - E_1^0} = -\frac{A^2}{2\varepsilon}$$

Therefore, the energies corrected upto second order

$$E_1 = E_0 + \varepsilon + \frac{A^2}{2\varepsilon}, \qquad E_2 = E_0 - \varepsilon - \frac{A^2}{2\varepsilon}$$

The wave function corrected to first order is given by

$$\psi_n = \psi_n^0 + \sum_m \frac{\langle m|H'|n\rangle}{E_n^0 - E_m^0}|\psi_m^0\rangle$$

$$\psi_1 = |\phi_1\rangle + \frac{\langle 1|H'|2\rangle}{E_1^0 - E_2^0}|\phi_2\rangle = |\phi_1\rangle + \frac{A}{E_1^0 - E_2^0}|\phi_2\rangle = |\phi_1\rangle + \frac{A}{2\varepsilon}|\phi_2\rangle$$

$$\psi_2 = |\phi_2\rangle + \frac{\langle 2|H'|1\rangle}{E_2^0 - E_1^0}|\phi_1\rangle = |\phi_2\rangle + \frac{A}{E_2^0 - E_1^0}|\phi_1\rangle = |\phi_2\rangle - \frac{A}{2\varepsilon}|\phi_1\rangle$$

Example 8. A system described by the Hamiltonian $H = \alpha L^2$, where L^2 is the square of the angular momentum and α is a constant, exhibits a line spectrum where the line A represents transition from the second excited state to the first excited state. The system is now placed in an external magnetic field and the Hamiltonian changes to $H = \alpha L^2 + \beta L_z$, where L_z is the z-component of the angular momentum. How many distinct lines will the original line A split into?

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Soln. The normalized eigenkets of the unperturbed Hamiltonian $H = \alpha L^2$ are $|\ell m\rangle$, where $l = 0, 1, 2, \ldots\ldots$, $m = 0, \pm 1, \pm 2, \ldots\ldots$.

For the first excited state $\ell = 1, m = 0, \pm 1$ and the second excited state $\ell = 2, m = 0, \pm 1, \pm 2$.

In the presence of magnetic field, $H = \alpha L^2 + \beta L_z$. So, the perturbing Hamiltonian is $H' = \beta L_z$

First order correction to energy in the state $|lm\rangle = \langle \ell m|\beta L_z|lm\rangle = \beta m\hbar$ for a given value of ℓ.

For the first excited state, the first order correction to energy $= \beta m\hbar = \beta\hbar, 0, -\beta\hbar$

For the second excited state, the first order correction to energy $= \beta m\hbar = 2\beta\hbar, \beta\hbar, 0, -\beta\hbar, -2\beta\hbar$

Figure below illustrates the splitting of the two energy levels. The allowed transitions will be

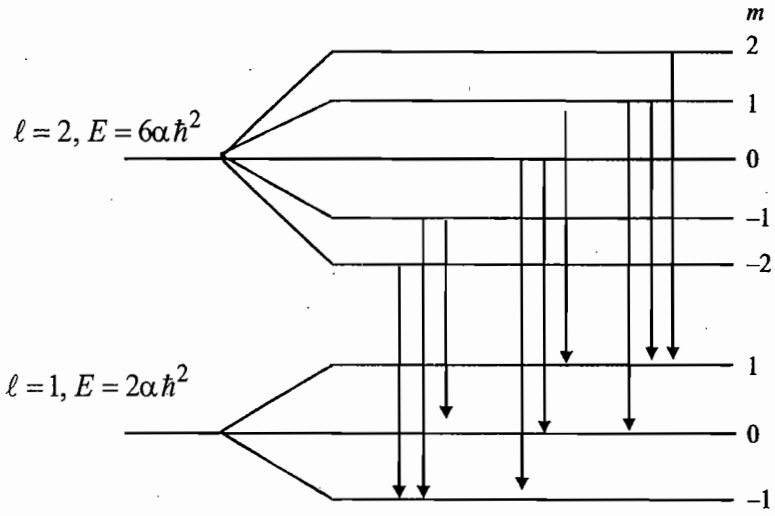

Figure: Transitions in the presence of magnetic field.

Example 9. The Hamiltonian of a two-electron system is perturbed by an interaction $\alpha \vec{S}_1.\vec{S}_2$, where α is a constant and $\vec{S}_1$ and $\vec{S}_2$ are the spin angular momenta of the electrons. Calculate the splitting between the S = 0 and S = 1 states by first order perturbation, where S is the magnitude of the total spin.

Soln. We have $\vec{S} = \vec{S}_1 + \vec{S}_2$. Then,

$$S^2 = S_1^2 + S_2^2 + 2\vec{S}_1.\vec{S}_2 \Rightarrow \vec{S}_1.\vec{S}_2 = \frac{S^2 - S_1^2 - S_2^2}{2}$$

Since the spin of electron is 1/2 when the two electrons combine, the total spin S = 0 or 1.
The state, for which S = 0 is called a singlet state with $m_s = 0$.
The state, for which S = 1 is called a triplet state with $m_s = 1, 0, -1$.
The first order correction to S = 0 state in the $|sm_s\rangle$ basis is

$$E_0^{(1)} = \left\langle sm_s \left| \frac{S^2 - S_1^2 - S_2^2}{2} \right| sm_s \right\rangle$$

$$= \frac{\alpha}{2}\left[s(s+1) - s_1(s_1+1) - s_2(s_2+1)\right]\hbar^2 = \frac{\alpha}{2}\left[0 - \frac{3}{4} - \frac{3}{4}\right]\hbar^2 = -\frac{3}{4}a\hbar^2$$

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The first order correction to the S = 1 state in the $|sm_s\rangle$ basis is

$$E_1^{(1)} = \frac{\alpha}{2}\left[1\times 2 - \frac{1}{2}\times\frac{3}{2} - \frac{1}{2}\times\frac{3}{2}\right]\hbar^2 = \frac{\alpha}{4}\hbar^2$$

Splitting between the two states $= \frac{\alpha}{4}\hbar^2 - \left(-\frac{3}{4}a\hbar^2\right) = \alpha\hbar^2$

Example 10. Consider an atomic state specified by angular momenta $\vec{L}, S$ and $\vec{J} = \vec{L} + \vec{S}$ placed in a magnetic field $\vec{B}$. Treating the interaction representing the magnetic moment of the electron in the magnetic field as the perturbing Hamiltonian and writing $\vec{L} + 2\vec{S} = g_J\vec{J}$, obtain an expression for (i) the g factor of the Jth state are (ii) the corrected energy.

Soln. When placed in the magnetic field $\vec{B}$, the interaction Hamiltonian

$$H' = -\vec{\mu}.\vec{B} = -(\vec{\mu}_L + \vec{\mu}_S).\vec{B} = \frac{e}{2m}(\vec{L} + 2\vec{S}).\vec{B}$$

where μ_L and μ_S are the orbital and spin magnetic moments of the electron.

Using, $g_J J = \vec{L} + 2\vec{S}$, we get the interaction Hamiltonian

$$H' = \frac{e}{2m} g_J \vec{J}.\vec{B} = \frac{e}{2m} g_J B J_z$$

The first order correction to the energy due to interaction Hamiltonian

$$E^{(1)} = \frac{e}{2m} g_J B m_j \hbar = \frac{e\hbar}{2m} B g_J m_j$$

The corrected energy $E = E^0 + \frac{e\hbar}{2m} B g_J m_j$

Since m_j can have $(2J+1)$-fold degenerate, each energy level is split into $2J+1$ equally spaced levels.

Example 11. A simple pendulum of length 'l' swings in a vertical plane under the influence of gravity. In the small angle approximation, find the energy levels of the system. Also evaluate the first order correction to the ground state energy, taking one more term in the small angle approximation.

Soln. The energy eigenvalues and eigenfunctions are the same as those of a linear harmonic oscillator with anglar frequency $\omega = \sqrt{g/\ell}$, where l is the length of the pendulum. While evaluating the energy eigenvalues, we assumed the angle θ to be small and retained only two terms in the expansion of $\cos\theta$. Retaining one more term, we get

$$\cos\theta = 1 - \frac{\theta^2}{2} + \frac{\theta^4}{24}$$

Then, the form of the potential will be

$$V = mg\ell(1-\cos\theta) = mg\ell\left(\frac{\theta^2}{2} - \frac{\theta^4}{24}\right) = \frac{mg\ell\theta^2}{2} - \frac{mg\ell\theta^4}{24}$$

Since $\theta = x/\ell$, then the Perturbing Hamiltonian $H' = -\frac{mg\ell\theta^4}{24} = -\frac{mgx^4}{24\ell^3}$

The first order correction to the ground state energy is

$$E_0^{(1)} = \left\langle 0\left| -\frac{mgx^4}{24\ell^3}\right| 0\right\rangle = \left(-\frac{mg}{24\ell^3}\right)\left(\frac{\hbar}{2m\omega}\right)^2 \left\langle 0\left|\left(a+a^\dagger\right)\left(a+a^\dagger\right)\left(a+a^\dagger\right)\left(a+a^\dagger\right)\right|0\right\rangle$$

In all, there will be 16 terms on the RHS. However, only two will be non-vanishing. They are

$$\left\langle 0\left|aa^\dagger aa^\dagger\right|0\right\rangle = 1, \qquad \left\langle 0\left|aaa^\dagger a^\dagger\right|0\right\rangle = 2$$

Hence, the first order correction to energy will be $E_0^{(1)} = -\frac{g\hbar^2}{8m\ell^3\omega^2}$

Example 12. Obtain the hyperfine splitting in the ground state of the hydrogen atom to first order in perturbation theory, for the perturbation

$$H'_{mn} = \langle \varphi_m | \hat{H}' | \varphi_n \rangle, \quad A \text{ being constant.}$$

where $\vec{S}_p$ and $\vec{S}_e$ denote the spins of the proton and electron, respectively.

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Soln. The hydrogen ground state wave function is

$$\psi_{100} = \left(\frac{1}{\pi a_0^3}\right)^{1/2} e^{-r/a_0}$$

Denoting the spin function by χ_s, the total wave function of the ground state is $\psi = \psi_{100}\chi_s$

The first order correction to energy

$$E_0^{(1)} = \left\langle \psi_{100}\chi_s \left| A\vec{S}_p.\vec{S}_e\delta^3(\vec{r}) \right| \psi_{100}\chi_s \right\rangle = \left\langle \psi_{100} \left| A\delta^3(\vec{r}) \right| \psi_{100} \right\rangle \left\langle \chi_s \left| \vec{S}_p.\vec{S}_e \right| \chi_s \right\rangle$$

$$= \frac{A}{\pi a_0^3} \left\langle \xi_s \left| \vec{S}_p.\vec{S}_e \right| \chi_s \right\rangle$$

$$= \frac{A}{\pi a_0^3} \left\langle \chi_s \left| \frac{F^2 - S_p^2 - S_e^2}{2} \right| \chi_s \right\rangle = \frac{A}{2\pi a_0^3} \left[F(F+1) - S_p(S_p+1) - S_e(S_e+1) \right] \hbar^2$$

As $S_p = \left(\frac{1}{2}\right)$ and $S_e = \left(\frac{1}{2}\right)$, the possible values of F are 1, 0.

The separation between the two F states is the hyperfine splitting ΔE. Thus,

$$\Delta E = \frac{A}{2\pi a_0^3} \left[\left(1\times 2 - \frac{1}{2}\times\frac{3}{2} - \frac{1}{2}\times\frac{3}{2} \right) - \left(0 - \frac{1}{2}\times\frac{3}{2} - \frac{1}{2}\times\frac{3}{2} \right) \right] \hbar^2 = \frac{A}{\pi a_0^3}\hbar^2$$

Example 13. The Hamiltonian matrix of a system in the orthonormal basis

$$\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

is given by

$$H = \begin{pmatrix} 1 & 2\varepsilon & 0 \\ 2\varepsilon & 2+\varepsilon & 3\varepsilon \\ 0 & 3\varepsilon & 3+\varepsilon \end{pmatrix}$$

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Find the energy levels corrected up to second order in the small parameter ε.

Soln. The matrix H can be written as

$$H = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 3 \end{pmatrix} + \begin{pmatrix} 0 & 2\varepsilon & 0 \\ 2\varepsilon & \varepsilon & 3\varepsilon \\ 0 & 3\varepsilon & \varepsilon \end{pmatrix} = H^0 + H'$$

Identifying H^0 and H' as the unperturbed and perturbation part, the eigenvalues of the unperturbed Hamiltonian H^0 are 1, 2 and 3. The first order correction to the energy is given by the diagonal matrix element of H'. Then,

$$H'_{11} = \langle 1|H'|1\rangle = (1\,0\,0) \begin{pmatrix} 0 & 2 & 0 \\ 2 & 1 & 3 \\ 0 & 3 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \varepsilon = 0$$

$$H'_{22} = \langle 2|H'|2\rangle = (0\,1\,0)\begin{pmatrix} 0 & 2 & 0 \\ 2 & 1 & 3 \\ 0 & 3 & 1 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}\varepsilon = \varepsilon$$

$$H'_{33} = \langle 3|H'|3\rangle = (0\,0\,1)\begin{pmatrix} 0 & 2 & 0 \\ 2 & 1 & 3 \\ 0 & 3 & 1 \end{pmatrix}\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}\varepsilon = \varepsilon$$

The first order correction to the energies are 0, ε, ε respectively. The second order correction is given by

$$E_n^{(2)} = \sum_m \frac{|\langle m|H'|n\rangle|^2}{E_n^0 - E_m^0}$$

$$H'_{12} = \langle 1|H'|2\rangle = (1\,0\,0)\begin{pmatrix} 0 & 2 & 0 \\ 2 & 1 & 3 \\ 0 & 3 & 1 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}\varepsilon = (1\,0\,0)\begin{pmatrix} 2 \\ 1 \\ 3 \end{pmatrix}\varepsilon = 2\varepsilon$$

$$H'_{13} = \langle 1|H'|3\rangle = (1\,0\,0)\begin{pmatrix} 0 & 2 & 0 \\ 2 & 1 & 3 \\ 0 & 3 & 1 \end{pmatrix}\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}\varepsilon = (1\,0\,0)\begin{pmatrix} 0 \\ 3 \\ 1 \end{pmatrix}\varepsilon = 0$$

$$H'_{23} = \langle 2|H'|3\rangle = (0\,1\,0)\begin{pmatrix} 0 & 2 & 0 \\ 2 & 1 & 3 \\ 0 & 3 & 1 \end{pmatrix}\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}\varepsilon = (0\,1\,0)\begin{pmatrix} 0 \\ 3 \\ 1 \end{pmatrix}\varepsilon = 3\varepsilon$$

$$E_1^{(2)} = \frac{|H'_{12}|^2}{E_1^{(0)} - E_2^{(0)}} + \frac{|H'_{13}|^2}{E_1^{(0)} - E_3^{(0)}} = \frac{|H'_{21}|^2}{1-2} + \frac{|H'_{31}|^2}{1-3} = -4\varepsilon^2 + 0 = -4\varepsilon^2$$

$$E_2^{(2)} = \frac{|H'_{12}|^2}{E_2^{(0)} - E_1^{(0)}} + \frac{|H'_{32}|^2}{E_2^{(0)} - E_3^{(0)}} = \frac{|H'_{12}|^2}{2-1} + \frac{|H'_{32}|^2}{2-3} = 4\varepsilon^2 - 9\varepsilon^2 = -5\varepsilon^2$$

$$E_3^{(2)} = \frac{|H'_{13}|^2}{E_3^{(0)} - E_1^{(0)}} + \frac{|H'_{23}|^2}{E_3^{(0)} - E_2^{(0)}} = \frac{|H'_{13}|^2}{3-1} + \frac{|H'_{23}|^2}{3-2} = 0 + 9\varepsilon^2 = 9\varepsilon^2$$

The energies of the three levels corrected to second order are

$$E_1 = 1 + 0 - 4\varepsilon^2 = 1 - 4\varepsilon^2$$

$$E_2 = 2 + \varepsilon - 5\varepsilon^2$$

$$E_3 = 3 + \varepsilon + 9\varepsilon^2$$

Degenerate Perturbation Theory :

In the time independent perturbation approach, the Hamiltonian of the system can be written as

$$\hat{H} = \hat{H}_0 + \hat{H}'$$

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where $\hat{H}_0$ is the unperturbed Hamiltonian. Here, the energy eigenvalue of the n[th] state i.e. E_n^0 is f-fold degenerate and the corresponding degenerate eigenfunctions are $|\varphi_1\rangle, |\varphi_2\rangle, \ldots\ldots |\varphi_f\rangle$ respectively.

Suppose the energy correction due to the perturbation $\hat{H}'$ is $E_n^{(1)}$, then $E_n^{(1)}$ can be calculated by solving the following equation containing secular determinant on the left hand side:

given

$$\begin{vmatrix} H'_{11} - E_n^{(1)} & H'_{12} & \ldots. & \ldots. & H'_{1f} \\ H'_{21} & H'_{22} - E_n^{(1)} & \ldots. & \ldots. & H'_{2f} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ H'_{f1} & H'_{f2} & \ldots. & \ldots. & H'_{ff} - E_n^{(1)} \end{vmatrix} = 0$$

where $H'_{mn} = \langle \varphi_m | \hat{H}' | \varphi_n \rangle$.

Example 14. The Hamiltonian matrix of a system is

$$H = \begin{pmatrix} 1 & \varepsilon & 0 \\ \varepsilon & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}, \qquad \varepsilon << 1$$

Find the energy eigenvalues corrected to first order in the perturbation. Also, find the eigenkets if the unperturbed eigenvalues are $|\phi_1\rangle$, $|\phi_2\rangle$ and $|\phi_3\rangle$.

Soln. The Hamiltonian matrix can be written as

$$H = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix} + \begin{pmatrix} 0 & \varepsilon & 0 \\ \varepsilon & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = H_0 + H'$$

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The energy eogenvalues of the unperturbed Hamiltonian are 1, 1, 2 units. Therefore, the energy 1 units are two-fold degenerate. The secular determinant corresponding to H' is

$$\begin{vmatrix} -E_n^{(1)} & \varepsilon & 0 \\ \varepsilon & -E_n^{(1)} & 0 \\ 0 & 0 & -E_n^{(1)} \end{vmatrix} = 0 \quad \Rightarrow E_n^{(1)} \left[\left\{ E_n^{(1)} \right\}^2 - \varepsilon^2 \right] = 0 \quad \Rightarrow E_n^{(1)} = \varepsilon, -\varepsilon, 0$$

where $E_n^{(1)}$ is the first order correction. The solution gives $E_n^{(1)} = \varepsilon, -\varepsilon, 0$

Suppose, $|\varphi_1\rangle, |\varphi_2\rangle, |\varphi_3\rangle$ are eigenkets of the unperturbed hamiltonian. Here, the state $|\phi_3\rangle$ is not affected by the perturbation. The eigenkets corresponding to states 1 and 2 can easily be obtained. Let these states be

$$|\phi'_n\rangle = c_1 |\phi_1\rangle + c_2 |\phi_2\rangle, \ [n = 1, 2]$$

where $|\varphi_n'\rangle$ is the eigenfunction of the perturbing hamiltonian H'.

The coefficients of eigenfunction $|\varphi_n'\rangle$ must obey the condition $-E_n^{(1)}c_1 + \varepsilon c_2 = 0$

For the eigenvalue $E_n^{(1)} = \varepsilon$, this equation reduces to $-\varepsilon c_1 + \varepsilon c_2 = 0$ or $c_1 = c_2$

Normalization of eigenfunction $|\varphi_n'\rangle$ gives $c_1 = c_2 = 1/\sqrt{2}$. Hence,

$$\phi'_1 = \frac{1}{\sqrt{2}}\left[|\phi_1\rangle + |\phi_2\rangle\right]$$

For the eigenvalue $E_n^{(1)} = -\varepsilon$, $\varepsilon c_1 + \varepsilon c_2 = 0$ or $c_1 = -c_2$

Normalization of eigenfunction $|\varphi_n'\rangle$ gives $c_1 = -c_2 = 1/\sqrt{2}$. This leads to

$$\phi'_2 = \frac{1}{\sqrt{2}}\left[|\phi_1\rangle - |\phi_2\rangle\right]$$

Thus, the corrected energies and eigenkets are

$$E_n' = 1-\varepsilon; \quad |\varphi_n'\rangle = \frac{1}{\sqrt{2}}\left[|\phi_1\rangle + |\phi_2\rangle\right]$$

$$E_n' = 1+\varepsilon; \quad |\varphi_n'\rangle = \frac{1}{\sqrt{2}}\left[|\phi_1\rangle - |\phi_2\rangle\right]$$

$$E_n' = 2; \quad |\varphi_n'\rangle = |\phi_3\rangle$$

Example 15. A hydrogen atom in the first excited state is placed in a uniform electric field ε along the positive z-axis. Evaluate the second order correction to the energy. Draw an energy level diagram illustrating the different states in the presence of the field. Given

$$\psi_{200} = \frac{1}{\pi^{1/2}}\left(\frac{1}{2a_0}\right)^{3/2}\left(1-\frac{r}{2a_0}\right)e^{-r/2a_0}$$

$$\psi_{210} = \frac{1}{\pi^{1/2}}\left(\frac{1}{2a_0}\right)^{5/2} re^{-r/2a_0}\cos\theta$$

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$$\int_0^\infty x^n e^{-ax}dx = \frac{n!}{a^{n+1}}$$

Soln. The first excited state (n = 2) is four-fold degenerate. The possible (ℓ, m) values are (0, 0), (1, 0), (1, –1). The four degerate states are $|n\ell m\rangle : |200\rangle, |210\rangle, |211\rangle$ and $|21,-1\rangle$. The additional potential energy in the field can be taken as the perturbation, i.e.,

$$H' = er\varepsilon\cos\theta$$

The energy of the n = 2 state, E_2^0 is the unperturbed energy. Out of the 12 off-diagonal elements, in 10 we have the factor.

$$\int_0^{2\pi} e^{i(m'-m)\phi}\, d\phi$$

which is equal to zero if $m' \neq m$. Only two off-diagonal elements will be non-vanishing; these are

$$\langle 200|er\varepsilon\cos\theta|210\rangle = \frac{e\varepsilon}{16\pi a_0^4}\int_0^{2\pi}\int_0^{\pi}\int_0^{\infty}\left(1-\frac{r}{2a_0}\right) r^4 e^{-r/a_0}\cos^2\theta\sin\theta\, dr\, d\theta\, d\phi$$

$$= \frac{e\varepsilon 2\pi}{19\pi a_0^4}\int_0^{\pi}\cos^2\theta\sin\theta d\theta\int_0^{\infty}\left(r^4-\frac{r^5}{2a_0}\right)e^{-r/a_0}dr$$

The integral in θ is very straighforward. The integral in the variable 'r' can be evaluated with the data given. Then,

$$\int_0^{\pi}\cos^2\theta\sin\theta d\theta = \frac{2}{3}$$

$$\int_0^{\infty}\left(r^4-\frac{r^5}{2a_0}\right)e^{-r/a_0}dr = -36a_0^5$$

Therefre, $\langle 200|H'|210\rangle = \frac{e\varepsilon}{8a_0^4}\times\frac{2}{3}\left(36a_0^5\right) = -3ea_0\varepsilon$

Then the perturbation matrix is

$(n\ell m)\rightarrow$ (200) (210) (211) $(21,-1)$

$\downarrow$

$$\begin{array}{c} (200)\\(210)\\(211)\\(21,-1)\end{array}\begin{bmatrix} 0 & -3ea_0\varepsilon & 0 & 0\\ -3ea_0\varepsilon & 0 & 0 & 0\\ 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0\end{bmatrix}$$

and the secular determinant is

$$\begin{vmatrix} -E_2^{(1)} & -3ea_0\varepsilon & 0 & 0\\ -3ea_0\varepsilon & -E_2^{(1)} & 0 & 0\\ 0 & 0 & -E_2^{(1)} & 0\\ 0 & 0 & 0 & -E_2^{(1)}\end{vmatrix} = 0 \qquad \ldots (vii)$$

The four roots of this determinant are $3ea_0\varepsilon, -3ea_0\varepsilon, 0$ and 0. The states $|200\rangle$ and $|210\rangle$ are affected by the electric field, whereas the states $|211\rangle$ and $|21,-1\rangle$ are not. Including the correction, the energy of the states are

$$E_2^0 - 3ea_0\varepsilon, \quad E_2^0 \text{ and } E_2^0 + 3ea_0\varepsilon$$

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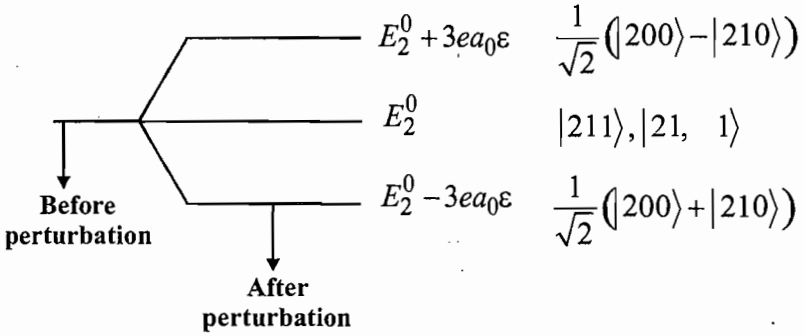

7.2. Time dependent perturbation theory :

In large number of quantum systems, the hamiltonian may also depend on time. In those systems, there will be no stationary states. The hamiltonian of such systems can be written as,

$$\hat{H}(t) = \hat{H}_0 + \hat{H}'(t) = \hat{H}_0 + \hat{H}_p(t)$$

where $\hat{H}_0$ is the time independent unperturbed hamiltonian and $\hat{H}_p(t)$ is the time dependent perturbing Hamiltonian such that $\hat{H}_p << \hat{H}_0$.

Suppose for the time interval $0 \le t \le \tau$, the system is subjected to extranal time-dependent perturbation $\hat{H}_p(t)$, which compared to H_0 i.e.

$$\hat{H}_p(t) = \hat{V}(t) \quad 0 \le t \le \tau$$
$$= 0 \quad \text{otherwise}$$

The corresponding time dependent Schrodinger equation is given by

$$i\hbar \frac{\partial \psi(\vec{r},t)}{\partial t} = \left[\hat{H}_0 + \hat{H}_p(t)\right]\psi(\vec{r},t) \Rightarrow i\hbar \frac{\partial \psi(\vec{r},t)}{\partial t} = \left[\hat{H}_0 + \hat{V}(t)\right]\psi(\vec{r},t)$$

where $\hat{V}(t)$ characterizes the interaction of the system with the external source of perturbation.

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Effect of $\hat{V}(t)$:

When the quantum mechanical system interacts with time dependent perturbation $\hat{V}(t)$, it either absorbs or emits energy external peturbation. This causes the system to undergo transitions from one unperturbed eigenstate of the Hamiltonian $\hat{H}_0$ to another unperturbed eigenstate of the Hamiltonian $\hat{H}_0$.

If the system is initially in an unperturbed eigenstate $|\psi_i\rangle$ of $\hat{H}_0$, then the probability that system will be found in an another unperturbed eigenstate $|\psi_f\rangle$, at a later time 't' will be

$$P_{if}(t) = \left| -\frac{i}{\hbar} \int_{t'=0}^{\infty} \langle \psi_f | \hat{V}(t') | \psi_i \rangle e^{i\omega_{fi}t'} dt' \right|^2$$

where, $\omega_{fi} = (E_f - E_i)/\hbar = \frac{1}{\hbar}\left[\langle \psi_f | \hat{H}_0 | \psi_f \rangle - \langle \psi_i | \hat{H}_0 | \psi_i \rangle\right]$

Constant Perturbation:

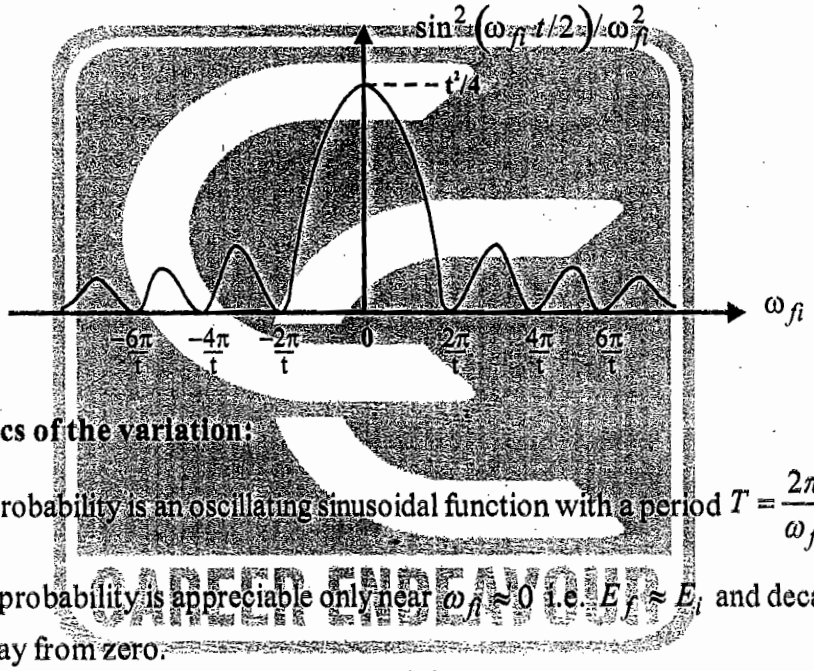
In this case, $\hat{V}(t)$ does not depend on time, therefore the transition probability will be

$$P_{if}(t)=\frac{1}{\hbar^2}\left|\left\langle\psi_f\left|\hat{V}\right|\psi_i\right\rangle\right|^2\left|\int_0^t e^{i\omega_{fi}t'}\,dt'\right|^2=\frac{1}{\hbar^2}\left|\left\langle\psi_f\left|\hat{V}\right|\psi_i\right\rangle\right|^2\left[\frac{e^{i\omega_{fi}t}-1}{i\omega_{fi}}\right]^2$$

$$=\frac{1}{\hbar^2}\frac{\left|\left\langle\psi_f\left|\hat{V}\right|\psi_i\right\rangle\right|^2\left|e^{i\omega_{fi}t/2}\right|^2\left|e^{i\omega_f t/2}-e^{-i\omega_{fi}t/2}\right|^2}{\omega_{fi}^2}=\frac{4\left|\left\langle\psi_f\left|\hat{V}\right|\psi_i\right\rangle\right|^2}{\hbar^2\psi_{fi}^2}\sin^2\left(\frac{\omega_{fi}t}{2}\right)$$

Therefore, $P_{if}(t)=\frac{\left|\left\langle\psi_f\left|\hat{V}\right|\psi_i\right\rangle\right|^2}{\hbar^2}t^2\frac{\sin^2(\omega_{fi}t/2)}{(\omega_{fi}t/2)^2}=\frac{\left|\left\langle\omega_f\left|\hat{V}\right|\psi_i\right\rangle\right|^2}{\hbar^2}t^2\,\mathrm{sinc}^2\left(\frac{\omega_{fi}t}{2}\right)$

Variation of the transition probability with the transition frequency:



Characteristics of the variation:

(i) Transition probability is an oscillating sinusoidal function with a period $T=\frac{2\pi}{\omega_{fi}}$

(ii) Transition probability is appreciable only near $\omega_{fi}\approx 0$ i.e. $E_f\approx E_i$ and decays rapidly as ω_{fi} moves away from zero.

(iii) The height and width of the main peak is proportional to t^2 and $1/t$. So, area under the curve is proportional to t. Therefore, transition probability grows linearly with time.

(iv) As time increases, the central peak becomes narrower and higher and in the limit $t\to\infty$, the transition probability takes the shape dirac delta function i.e.

$$P_{if}(t)=\frac{2\pi t}{\hbar}\left|\left\langle\psi_f\left|\hat{V}\right|\psi_i\right\rangle\right|^2\delta(E_f-E_i)$$

(v) Transition rate = transition probability per unit time is given by

$$\tau_{if}=\frac{P_{if}(t)}{t}=\frac{2\pi}{\hbar}\left|\left\langle\psi_f\left|\hat{V}\right|\psi_i\right\rangle\right|^2\delta(E_f-E_i)$$

i.e. transition rate is non-vanishing only between states of equal energy. Hence, a constant perturbation neither removes energy from the system nor supplies energy to the system. This causes energy conserved transition.

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Fermi Golden Rule:

Consider a transition from an initial state $|\psi_i\rangle$ into a continuum of final states $|\psi_f\rangle$. If $\rho(E_f)$ is density of final states i.e. number of final states per unit energy interval, then number of final states within the energy interval E_f to $E_f + dE_f$ is equal to $\rho(E_f)dE_f$.

Therefore, total transition rate

$$W_{if} = \int \frac{P_{if}(t)}{t}\rho(E_f)dE_f$$

$$= \frac{2\pi}{\hbar}\left|\langle\omega_f|\hat{V}|\psi_i\rangle\right|^2 \int \rho(E_f)\,\delta(E_f - E_i)\,dE_f \;= \frac{2\pi}{\hbar}\left|\langle\omega_f|\hat{V}|\psi_i\rangle\right|^2 \rho(E_i)$$

This relation is called Fermi golden rule i.e for a constant perturbation, if we wait long enough, total transition rate becomes constant.

Harmonic Perturbation:

Consider the following harmonic perturbation:

$$\hat{V}(t) = \hat{v}e^{i\omega t} + \hat{v}^{\dagger}e^{-i\omega t}$$

where $\hat{v}$ and $\hat{v}^{\dagger}$ are time independent operator.

Such a perturbation is encountered, when charged particles (i.e. electrons) interach with an electromagnetic field. This perturbation envokes transitions of the system from one staionary state to another. The corresponding transition probability will be

$$P_{if}(t) = \frac{1}{\hbar^2}\left|\langle\psi_f|\hat{v}|\psi_i\rangle\int_0^t e^{i(\omega_{fi}+\omega)t'}dt + \langle\psi_f|\hat{v}^{\dagger}|\psi_i\rangle\int_0^t e^{i(\omega_{fi}-\omega)t'}dt'\right|^2$$

Neglecting the cross terms, we can write

$$\Rightarrow \quad P_{if}(t) = \frac{1}{\hbar^2}\left|\langle\psi_f|\hat{v}|\psi_i\rangle\right|^2\left|\frac{e^{i(\omega_{fi}+\omega)t}-1}{i(\omega_{fi}+\omega)}\right|^2 + \frac{1}{\hbar^2}\left|\langle\psi_f|\hat{v}^{\dagger}|\psi_i\rangle\right|^2\left|\frac{e^{i(\omega_{fi}-\omega)t}-1}{i(\omega_{fi}-\omega)}\right|^2$$

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$$\Rightarrow \quad P_{if}(t) = \frac{4}{\hbar^2}\left[\left|\langle\psi_f|\hat{v}|\psi_i\rangle\right|^2\frac{\sin^2\{(\omega_{fi}+\omega)t/2\}}{(\omega_{fi}+\omega)^2} + \left|\langle\psi_f|\hat{v}^{\dagger}|\psi_i\rangle\right|^2\frac{\sin^2\{(\omega_{fi}-\omega)t/2\}}{(\omega_{fi}-\omega)^2}\right]$$

Transition probability peaks at

(i) $\omega_{fi} = -\omega \quad \Rightarrow \quad P_{if}(t)\big|_{\max} = \left(\frac{t^2}{4\hbar^2}\right)\left|\langle\psi_f|\hat{v}|\psi_i\rangle\right|^2$

(ii) $\omega_{fi} = \omega \quad \Rightarrow \quad P_{if}(t)\big|_{\max} = \left(\frac{t^2}{4\hbar^2}\right)\left|\langle\psi_f|\hat{v}^{\dagger}|\psi_i\rangle\right|^2$

These corresponds to resonance i.e. transition probability will be maximumwhen frequency of the perturbing field is close to $\pm\omega_{fi}$.

Similarly as before as $t \to \infty$, the transition rate becomes

$$\Gamma_{if}(t) = \frac{2\pi}{\hbar}\left[\left|\langle\psi_f|\hat{v}|\psi_i\rangle\right|^2 \delta\left(E_f - E_i + \hbar\omega\right) + \left|\langle\psi_f|\hat{v}^\dagger|\psi_i\rangle\right|^2 \delta\left(E_f - E_i - \hbar\omega\right)\right]$$

Transition rate Γ_{if} will be non-zero only, if $E_f = E_i + \hbar\omega$ or $E_f = E_i - \hbar\omega$

(i) $E_f = E_i - \hbar\omega \Rightarrow$ the system is initially excited and when it is acted upon by the perturbation, the system deexcites by giving up a photon energy $\hbar\omega$ to $\hat{V}(t)$ and ends up in an less excited state of energy E_f. This process is known as Stimulated Emission.

(ii) $E_f = E_i + \hbar\omega \Rightarrow$ the system is initially in a less excited state and when it is acted upon by the perturbation, the system absorbs a photon of energy $\hbar\omega$ from $\hat{V}(t)$ and ends up in an higher excited state of energy E_f. This process is known as Stimulated Absorption.

Notes:

(i) The term $e^{i\omega t}$ is responsible for emission of photon and the term $e^{-i\omega t}$, responsible for absorption of photon.

(ii) Harmonic perturbation is either transfering energy to the system or receiving energy from the sytsem, in the form of photon of energy $\hbar\omega$.

Adiabatic approximation:

If the system is initially in the n[th] state of the unperturbed Hamiltonian and the Hamitonian evolves slowly with time, at a later time t it will be found in the n[th] state of the new (instaneous) hamiltonian i.e. that the sytem will not make any transitions.

This approximation is valid only when time change in energy corresponding to perturbation, during one period of oscillation is very small compared to $\left|E_f - E_i\right|$

i.e. $\left|\frac{1}{\omega_{fi}}\frac{\partial}{\partial t}\langle\omega_f|\hat{V}(t)|\psi_i\rangle\right| << \left|E_f - E_i\right|$

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Sudden Approximation:

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If the system is initially in the n[th] state of the unperturbed Hamiltonian and the Hamitonian evolves suddenly with time, at a later time t it will be found in the m[th] state of the new (instaneous) hamiltonian with the corresponding probability

$$P_{mn} = \left|\langle\phi_m|\psi_n\rangle\right|^2$$

Example 16. A particle of mass 'm' having charge 'e', confined to a three-dimensional cubical box of side 2a, is acted on by an electric field.

$$E = E_0 e^{-at}, \quad t > 0$$

where a is a constant, in the x-direction. Calculate the probability that the charged particle in the ground state at t = 0 is excited to the first excited state by the time $t = \infty$.

Soln. The energy eigenfunctions and eigenvalues of a particle in a cubical box of side '2a' are given by

$$E_{n_x n_y n_z} = \frac{\pi^2\hbar^2}{8ma^2}\left(n_x^2 + n_y^2 + n_z^2\right) \quad \left(n_x, n_y, n_z = 1, 2, 3.....\right)$$

$$\Psi_{n_x n_y n_z} = \frac{1}{\sqrt{a^3}} \sin\frac{n_x \pi x}{2a} \sin\frac{n_y \pi y}{2a} \sin\frac{n_z \pi z}{2a} = \left| n_x n_y n_z \right\rangle$$

The ground state is $|111\rangle$ and the first excited states are $|211\rangle, |121\rangle, |112\rangle$. Since the electric field is along the x-axis, the dipole moment $\mu = ex$ and the perturbation are given by

$$H' = -\mu.E = -eE_0 x e^{-at}$$

The transition probability for a transition from state n to state 'm' is obtained as

$$P = \left| C_m^{(1)} \right|^2 = \frac{1}{\hbar^2} \left| \int_0^\infty H'_{mn} \exp(i\omega_{mn} t)\, dt \right|^2$$

where, $\omega_{mn} = (E_m - E_n)/\hbar$, $c_m^{(1)}$ and H'_{mn} is the transition moment.

$$H'_{mn} = \langle 111|H'|211\rangle = \left\langle 111 \left| -eE_0 x e^{-at} \right| 211 \right\rangle$$

$$= -eE_0 e^{-at} \langle 111|x|211\rangle$$

$$= \frac{-eE_0 e^{-at}}{a^3} \int_0^{2a} x \sin\frac{\pi x}{2a} \sin\frac{\pi x}{a}\, dx \int_0^{2a} \sin^2\frac{\pi y}{2a}\, dy \int_0^{2a} \sin^2\frac{\pi z}{2b}\, dz$$

$$= \frac{-eE_0 e^{-at}}{a^3} \left(\frac{32a^2}{9\pi^2} \right) \times a \times a = \frac{32aeE_0 e^{-at}}{9\pi^2}$$

$$\langle 111|H'|121\rangle = \frac{-eE_0 e^{-at}}{a^3} \int_0^{2a} x \sin^2\frac{\pi x}{2a}\, dx \int_0^{2a} \sin\frac{\pi y}{2a} \sin\frac{\pi y}{a}\, dy \int_0^{2a} \sin^2\frac{\pi z}{2a}\, dz = 0$$

Similary, $\langle 111|H'|112\rangle = 0$

$$\omega_{21} = \frac{E_2 - E_1}{\hbar} = \frac{\pi^2\hbar^2}{8ma^2}\left(2^2 + 1^2 + 1^2 - 1^2 - 1^2 - 1^2\right) = \frac{3\pi^2\hbar^2}{8ma^2}$$

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Consequently, $P = \left(\frac{32aeE_0}{9\pi^2\hbar} \right) \left| \int_0^\alpha \exp(-\alpha t + i\omega_{21} t)\, dt \right| = \left(\frac{32aeE_0}{9\pi^2\hbar} \right) \frac{1}{\alpha^2 + \omega_{21}^2}$

Example 17. A hydrogen atom in the ground state is subjected to an electric field

$$E = E_0 e^{-t/\tau}, t > 0, \qquad \tau \text{ being constant}$$

along the z-axis. Calculate the probability for transition to the (200) and (210) states when it is very large.

Soln. The interaction Hamiltonian

$$H' = -\mu.E = -\mu E \cos\theta = erE_0 e^{-t/\tau} \cos\theta$$

$$\psi_{100} = \left(\frac{1}{\pi a_0^3} \right) e^{-r/a_0}$$

$$\psi_{200} = \frac{1}{\pi^{1/2}}\left(\frac{1}{2a_0}\right)^{3/2}\left(1-\frac{r}{2a_0}\right)e^{-r/a_0}$$

$$\psi_{210} = \frac{1}{\pi^{1/2}}\left(\frac{1}{2a_0}\right)^{5/2} r\, e^{-r/2a_0}\cos\theta$$

The probability for transition from $n \to k$ state is

$$P_{n\to k} = \frac{1}{\hbar^2}\left|\int_0^t H'_{kn}(r,t)\exp(i\omega_{kn}t)\,dt\right|^2 \qquad \omega_{kn} = \frac{E_k - E_n}{\hbar}$$

(100) to (200) transition:

$$H'_{21}(t) = \langle 200|H'|100\rangle = \int \psi_{200}\left(erE_0e^{-t/\tau}\cos\theta\right)\psi_{100}\,d\tau$$

The θ-part of the integral is

$$\int_0^{\pi}\cos\theta\sin\theta\,d\theta = 0$$

Hence, H'_{21} is zero. Therefore, the probability $P_{n\to k} = 0$.

(100) to (210) transition:

$$H'_{21}(t) = \langle 200|H'|100\rangle = \frac{eE_0e^{-t/\tau}}{\pi 2^{5/2}a_0^4}\int_0^{\infty} r^4 e^{-3r/2a_0}dr\int_0^{\pi}\cos^2\theta\sin\theta\,d\theta\int_0^{2\pi}d\phi$$

Writing $y = \cos\theta$, $dy = -\sin\theta\,d\theta$

We have, $\int_0^{\pi}\cos^2\theta\sin\theta\,d\theta = -\int_1^{-1}y^2dy = \frac{2}{3}$

$$H'_{21}(t) = \frac{eE_0e^{-t/\tau}}{\pi 2^{5/2}a_0^4}\times\frac{4!}{(3/2a_0)^5}\times\frac{2}{3}\times 2\pi = \frac{256eE_0a_0e^{-t/\tau}}{243\times\sqrt{2}}$$

where, $A = \frac{256eE_0a_0}{243\times\sqrt{2}}$

$$\int_0^t H'_{21}e^{i\omega t_{21}t}dt = A\int_0^t e^{-t/\tau}e^{i\omega t_{21}t}dt = A\int_0^t e^{-t/\tau}\left(\cos\omega_{21}t + i\sin\omega_{21}t\right)dt$$

As 't' is very large, we can assume the limits of integral as 0 to ∞. Then,

$$\int_0^{\infty} H'_{21}e^{i\omega_{21}t}dt = A\left(\frac{1/\tau}{\left(1/\tau^2\right)+\omega_{21}^2} + i\frac{\omega_{21}}{\left(1/\tau^2\right)+\omega_{21}^2}\right)$$

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$$P_{1\to 2}=\frac{A^2}{\hbar^2}\left(\frac{1/\tau}{\left(1/\tau^2\right)+\varepsilon_{21}^2}+i\frac{\omega_{21}}{\left(1/\tau^2\right)+\omega_{21}^2}\right)\left(\frac{1/\tau}{\left(1/\tau^2\right)+\omega_{21}^2}-i\frac{\omega_{21}}{\left(1/\tau^2\right)+\omega_{21}^2}\right)$$

CSIR PREVIOUS YEAR QUESTIONS

1. If the perturbation $H' = ax$, where a is a constant; is added to the infinite square well potential

$$V(x)=\begin{cases}0 \text{ for} & 0\le x\le \pi\\ \infty & \text{otherwise}\end{cases}$$

The first order correction to ground state energy is: **[CSIR June 2011]**

(a) $\frac{a\pi}{2}$ (b) $a\pi$ (c) $\frac{a\pi}{4}$ (d) $\frac{a\pi}{\sqrt{2}}$

Soln. For a infinite square well potential of width π, the ground state wave function will be

$$\psi_0(x)=\sqrt{\frac{2}{\pi}}\sin x$$

Given perturbation: $H' = ax$

First-order correction to the ground state $= \Delta E = \int_0^{\pi}\psi_0^* H\,\psi_0\,dx$

$$=\int_0^{\pi}\left(\frac{2}{\pi}\sin^2 x\right)ax\,dx=\frac{2a}{\pi}\int_0^{\pi}x\left(\sin^2 x\right)dx=\frac{2a}{\pi}\int_0^{\pi}x\left(\frac{1}{2}-\frac{1}{2}\cos 2x\right)dx$$

$$=\frac{a}{\pi}\left[\int_0^{\pi}x\,dx-\int_0^{\pi}x\cos 2x\,dx\right]=\frac{a}{\pi}\left[\frac{x^2}{2}\Big|_0^{\pi}-\left\{x\frac{\sin 2x}{2}\Big|_0^{\pi}-\int_0^{\pi}\frac{\sin 2x}{2}dx\right\}\right]$$

$$=\frac{a}{\pi}\left[\frac{\pi^2}{2}-\left\{0-\frac{1}{2}\frac{\cos 2x}{2}\Big|_0^{\pi}\right\}\right]=\frac{a\pi}{2}$$

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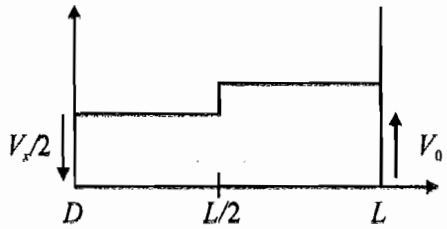
Correct answer is (a) www.careerendeavour.com

2. A constant perturbation as shown in the figure below acts on a particle of mass m confined in a infinite potential well between 0 and L.



The first-order correction to the ground state energy of the particle is **[CSIR Dec 2011]**

(a) $\frac{V_0}{2}$ (b) $\frac{3V_0}{4}$ (c) $\frac{V_0}{4}$ (d) $\frac{3V_0}{2}$

Soln. Ground state energy of the particle is given by

$$\psi_0 = \sqrt{\frac{2}{L}}\sin\left(\frac{\pi x}{L}\right)$$

First order correction to energy $= \Delta E = \int_0^L \psi_0^* H' \psi_0 dx$

$$= \int_0^{1/2}\left(\frac{2}{L}\right)\sin^2\left(\frac{\pi x}{L}\right)\frac{V_0}{2}dx + \int_{1/2}^{L}\left(\frac{2}{L}\right)\sin^2\left(\frac{\pi x}{L}\right)V_0 dx$$

$$= \frac{V_0}{L}\int_0^{1/2}\frac{\left(1-\cos\frac{2\pi x}{L}\right)}{2}dx + V_0\left(\frac{2}{L}\right)\int_{1/2}^{L}\frac{\left(1-\cos\frac{2\pi x}{L}\right)}{2}dx$$

$$\frac{V_0}{2L}\left[x - \frac{\sin\frac{2\pi x}{L}}{\frac{2\pi}{L}}\right]_0^{1/2} + \frac{V_0}{L}\left[x - \frac{\sin\frac{2\pi x}{L}}{\frac{2\pi}{L}}\right]_{1/2}^{L} = \frac{3V_0}{4}$$

Correct answer is (b)

3. The perturbation $H' = bx^4$, where 'b' is a constant, is added to the one dimensional harmonic oscillator potential $V(x) = \frac{1}{2}m\omega^2x^2$. Which of the following denotes the correction to the ground state energy to first order in b? **[CSIR Dec 2011]**

[Hint : The normalized ground state wave function of the one dimensional harmonic oscillator potential is $\psi_0 = \left(\frac{m\omega}{h\pi}\right)^{1/4} e^{-m\omega x^2/2\hbar}$. You may use the following integral $\int_{-\infty}^{\infty} x^{2n} e^{-ax^2}dx = a^{-n-\frac{1}{2}}\Gamma\left(n+\frac{1}{2}\right)$

(a) $\frac{3b\hbar^2}{4m^2\omega^2}$ (b) $\frac{3b\hbar^2}{2m^2\omega^2}$ (c) $\frac{3b\hbar^2}{2\pi m^2\omega^2}$ (d) $\frac{15b\hbar^2}{4m^2\omega^2}$

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Soln. First order correction to energy $= \Delta E = \int_{-\infty}^{\infty} \psi_0^* H' \psi_0 dx = b\left(\frac{m\omega}{\hbar\pi}\right)^{1/2}\int_{-\infty}^{\infty} e^{-\frac{m\omega x^2}{\hbar}} x^4 dx$

Using the standard given integral (for the above integral, $a = \frac{m\omega}{\hbar}$, $n = 2$), we get

$$\Delta E = b\left(\frac{m\omega}{\hbar\pi}\right)^{1/2}\left(\frac{m\omega}{\pi}\right)^{-2-1/2}\Gamma\left(2+\frac{1}{2}\right) = \frac{3b\hbar^2}{4m^2\omega^2}$$

Correct answer is (a)

4. Consider an electron in a box of lenght L with periodic boundary condition $\psi(x)=\psi(x+L)$. If the electron is in the $\psi_k(x)=\frac{1}{\sqrt{L}}e^{jkx}$ with energy $\varepsilon_k=\frac{\hbar^2k^2}{2m}$, what is the correction to its energy, to second order of perturbation theory, when it is subjected to weak periodic potential $V(x)=V_0\cos gx$, where g is an integral multiple of the $2\pi/L$? **[CSIR June 2012]**

(a) $V_0^2\,\varepsilon_g/\varepsilon_k^2$ (b) $-\frac{mV_0^2}{2\hbar^2}\left(\frac{1}{g^2+2kg}+\frac{1}{g^2-2kg}\right)$

(c) $V_0^2\left(\varepsilon_k-\varepsilon_g\right)/\varepsilon_g^2$ (d) $V_0^2/\left(\varepsilon_k+\varepsilon_g\right)$

Soln. Perturbed periodic potential, $V(x)=V_0\cos gx,\ \left[g=\frac{2m\pi}{L},\ m=1,2,3,4...\right]$

Second order correction to energy, $E_K^{(2)}=\sum_{K'\neq K}\frac{\left|\langle\psi_{K'}|V(x)|\psi_K\rangle\right|^2}{E_K-E_{K'}}$

$$\langle\psi_{K'}|V(x)|\psi_K\rangle=\int_0^L\psi_{K'}^*V_0\cos gx\,\psi_K\,dx$$

$$=\frac{V_0}{L}\int_0^L e^{-iK'x}\frac{\left(e^{igx}+e^{-igx}\right)}{2}e^{iKx}dx=\frac{V_0}{L}\left[\int_0^L e^{i(K+g-K')x}dx+\int_0^L e^{(K-g-K')x}dx\right]$$

$$=\frac{V_0}{2}\left[\delta\left(K+g-K'\right)+\delta\left(K-g-K'\right)\right]$$

Therefore, $E_K^{(2)}=\frac{\left|\langle\psi_{K+g}|V(x)|\psi_K\rangle\right|^2}{E_K-E_{K+g}}+\frac{\left|\langle\psi_{K-g}|V(x)|\psi_K\rangle\right|^2}{E_K-E_{K-g}}$

$$\Rightarrow E_K^{(2)}=\frac{\frac{V_0^2}{4}}{\frac{\hbar^2k^2}{2m}-\frac{\hbar^2(k+g)^2}{2m}}+\frac{\frac{V_0^2}{4}}{\frac{\hbar^2k^2}{2m}-\frac{\hbar^2(k-g)^2}{2m}}=-\frac{mV_0^2}{2\hbar^2}\left[\frac{1}{g^2+2kg}-\frac{1}{g^2-2kg}\right]$$

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Correct answer is (b).

5. The energy eigenvalues of a particle in the potential $V(x)=\frac{1}{2}m\omega^2x^2-ax$ are **[CSIR Dec 2012]**

(a) $E_n=\left(n+\frac{1}{2}\right)\hbar\omega-\frac{a^2}{2m\omega^2}$ (b) $E_n=\left(n+\frac{1}{2}\right)\hbar\omega+\frac{a^2}{2m\omega^2}$

(c) $E_n=\left(n+\frac{1}{2}\right)\hbar\omega-\frac{a^2}{m\omega^2}$ (d) $E_n=\left(n+\frac{1}{2}\right)\hbar\omega$

Soln. Perturbing Hamiltonian $=H_p=-ax$

First order correction to energy in the n^{th} state =

$$E_n^{(1)} = \langle n|H_p|n\rangle = -\langle n|ax|n\rangle = -\sqrt{\frac{\hbar}{2m\omega}}\left\langle n\left|\left(\hat{a}+\hat{a}^{\dagger}\right)\right|n\right\rangle = 0$$

Second order correction to energy $= E_n^{(2)} = \sum_{m\neq n}\frac{\left|\langle n|H'|m\rangle\right|^2}{E_n^0 - E_m^0}$

Now, $\langle n|H'|m\rangle = -a\sqrt{\frac{\hbar}{2m\omega}}\left\langle n\left|\hat{a}+\hat{a}^{\dagger}\right|m\right\rangle$

Here, m can take all integral values except n. The non-vanishing elements corresponds to $m=(n+1)$ and $(n-1)$. Hence,

Therefore, $E_n^{(2)} = a^2\frac{\hbar}{2m\omega}\left[\frac{\left(\sqrt{n+1}\right)^2}{E_n - E_{n+1}} + \frac{\left(\sqrt{n}\right)^2}{E_n - E_{n-1}}\right] = a^2\frac{\hbar}{2m\omega}\left[\frac{\left(\sqrt{n+1}\right)^2}{-\hbar\omega} + \frac{\left(\sqrt{n}\right)^2}{\hbar\omega}\right] = -\frac{a^2}{2m\omega^2}$

The energy eigenvalues corresponding to the given potential will be

$$E_n = \left(n+\frac{1}{2}\right)\hbar\omega - \frac{a^2}{2m\omega^2}$$

Correct option is (a)

6. The perturbation

$$H' = \begin{cases} b(a-x) & -a < x < a \\ 0 & \text{otherwise} \end{cases}$$

acts on a particle of mass 'm' confined in an infinite square well potential

$$V(x) = \begin{cases} 0 & -a < x < a \\ \infty & \text{otherwise} \end{cases}$$

The first order correction to the ground state energy of the particle is

(a) $\frac{ba}{2}$ (b) $\frac{ba}{\sqrt{2}}$ (c) $2ba$ (d) ba

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Soln. The ground state wavefunction for the given potential $\psi_1(x) = \sqrt{\frac{2}{2a}}\cos\left(\frac{\pi x}{2a}\right) = \frac{1}{\sqrt{a}}\cos\left(\frac{\pi x}{2a}\right)$

The first order correction in energy,

$$E' = \int \psi_1^* H'\psi_1 dx = \frac{b}{a}\int_{-a}^{+a}\cos^2\left(\frac{\pi x}{2a}\right)(a-x)\,dx$$

$$= \frac{b}{a}\int_{-a}^{+a}\frac{\left(1+\cos\frac{\pi x}{a}\right)}{2}(a-x)\,dx = \frac{b}{2a}\left[\int_{-a}^{+a}(a-x)\,dx + \int_{-a}^{+a}a\cos\frac{\pi x}{a}dx - \int_{-a}^{+a}x\cos\frac{\pi x}{a}dx\right]$$

$$= \frac{b}{2a}\left[\left\{ax - \frac{x^2}{2}\right\} + \frac{a\sin\left(\frac{\pi x}{a}\right)}{\frac{\pi}{a}}\right]_{-a}^{+a} = \frac{b}{2a}\left[2a^2 + 0\right] = ab$$

Correct option is (d)

7. Consider a two-dimensional infinite square will $V(x,y) = \begin{cases} 0 & 0 < x < a, \quad 0 < y < a \\ \infty & \text{otherwise} \end{cases}$. Its normalized eigenfunctions are $\psi_{n_x,n_y}(x,y) = \frac{2}{a}\sin\left(\frac{n_x \pi x}{a}\right)\sin\left(\frac{n_y \pi y}{a}\right)$ where n_x, n_y = 1, 2, 3, ... If a perturbation $H' = \begin{cases} V_0 & 0 < x < \frac{a}{2}, \quad 0 < y < \frac{a}{2} \\ 0 & \text{otherwise} \end{cases}$ is applied, then the correction to the energy of the first excited state to order V_0 is **[CSIR June 2013]**

(a) $\frac{V_0}{4}$ (b) $\frac{V_0}{4}\left[1 \pm \frac{64}{9\pi^2}\right]$ (c) $\frac{V_0}{4}\left[1 \pm \frac{16}{9\pi^2}\right]$ (d) $\frac{V_0}{4}\left[1 \pm \frac{32}{9\pi^2}\right]$

Soln. The energy of n^{th} state for 2-dimensional infinite squrae well

$$E_n = \frac{n_x^2\pi^2\hbar^2}{2ma^2} + \frac{n_y^2\pi^2\hbar^2}{2ma^2} \quad \text{... (i)}$$

The energy of first excited state $= \frac{5\pi^2\hbar^2}{2ma^2}$

and state is 2 fold degenerate with $(n_x, n_y) = (1,2)$ & $(2,1)$

To find first order corection in every of first excited state we use degenerate perturbation theory. We construct secular determinant

$$\begin{vmatrix} \langle\phi_1|H_P|\phi_1\rangle - E' & \langle\phi_1|H_P|\phi_2\rangle \\ \langle\phi_2|H_P|\phi_1\rangle & \langle\phi_2|H_P|\phi_2\rangle - E' \end{vmatrix} = 0 \quad \text{(ii)}$$

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Where, $\phi_1 = \frac{2}{a}\sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{2\pi y}{a}\right)$ and $\phi_2 = \frac{2}{a}\sin\left(\frac{2\pi x}{a}\right)\sin\left(\frac{\pi y}{a}\right)$

$$\langle\phi_1|H_P|\phi_1\rangle = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\phi_1^*(x,y)\,H_P\,\phi_1(x,y)\,dx\,dy$$

$$= V_0\int_0^{a/2}\frac{2}{a}\sin^2\left(\frac{\pi x}{a}\right)dx\int_0^{a/2}\sin^2\left(\frac{2\pi y}{a}\right)dy = \frac{V_0}{4}$$

Similarly, $\langle\phi_2|H_P|\phi_2\rangle = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\phi_2^*(x,y)\,H_P\phi_2(x,y)\,dxdy = \frac{V_0}{4}$

$$\langle\phi_1|H_P|\phi_2\rangle = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\phi_1^*(x,y)\,H_P\phi_2(x,y)\,dxdy$$

$$= V_0\int_0^{a/2}\int_0^{a/2}\left(\frac{2}{a}\right)^2\sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{2\pi y}{a}\right)\sin\left(\frac{2\pi x}{a}\right)\sin\left(\frac{\pi y}{a}\right)dxdy$$

$$= \frac{V_0}{a^2}\left[\int_0^{a/2} 2\sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{2\pi x}{a}\right)dx \int_0^{a/2} 2\sin\left(\frac{2\pi y}{a}\right)\sin\left(\frac{\pi y}{a}\right)dy\right]$$

$$= V_0 \frac{4}{3\pi} \times \frac{4}{3\pi} = \frac{16V_0}{9\pi^2}$$

on substituting these values of matrix elements in secular determinant.

$$\begin{vmatrix} \frac{V_0}{4} - E' & \frac{16V_0}{9\pi^2} \\ \frac{16V_0}{9\pi^2} & \frac{V_0}{4} - E' \end{vmatrix} = 0 \quad \Rightarrow \quad \left(\frac{V_0}{4} - E'\right)^2 - \left(\frac{16V_0}{9\pi^2}\right)^2 = 0$$

$$\Rightarrow \quad \frac{V_0}{4} - E' = \pm\frac{16V_0}{9\pi^2} \quad \Rightarrow \quad E' = \frac{V_0}{4} \pm \frac{16V_0}{9\pi^2} = \frac{V_0}{4}\left[1 \pm \frac{64}{9\pi^2}\right]$$

Correct answer is (b)

8. The motion of a particle of mass m in one dimension is described by the Hamiltonian $H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 + \lambda x$. What is the difference between the (quantized) energies of the first two levels? (In the following, $\langle x \rangle$ is the expectation value of x in the ground state)

[CSIR Dec 2013]

(a) $\hbar\omega - \lambda\langle x\rangle$ (b) $\hbar\omega + \lambda\langle x\rangle$ (c) $\hbar\omega + \frac{\lambda^2}{2m\omega^2}$ (d) $\hbar\omega$

Soln. Given : Hamiltonian of the system $H = \underbrace{\frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2}_{\text{Unperturbed Hamiltonian}} + \underbrace{\lambda x}_{\text{Perturbed Hamiltonian}}$

First order correction to energy of the n[th] state.

$$E_n^{(1)} = \langle n|\lambda x|n\rangle = \lambda\sqrt{\frac{\hbar}{2m\omega}}\langle n|\left(\hat{a} + \hat{a}^\dagger\right)|n\rangle = 0$$

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Second order correction to energy of the n[th] state.

$$E_n^{(2)} = \sum_{m\neq n} \frac{|\langle n|\lambda x|m\rangle|^2}{E_n^{(0)} - E_m^{(0)}} = \lambda^2 \frac{\hbar}{2m\omega} \sum_{m\neq n} \frac{\left|\left\langle n\left|\left(\hat{a} + \hat{a}^\dagger\right)\right|m\right\rangle\right|^2}{E_n^{(0)} - E_m^{(0)}}$$

The non-zero contribution comes only from $m = (n+1)$ and $(n-1)$

$$\Rightarrow \quad E_n^{(2)} = \frac{\lambda^2\hbar}{2m\omega}\left[\frac{\left(\sqrt{n+1}\right)^2}{-\hbar\omega} + \frac{\left(\sqrt{n}\right)^2}{\hbar\omega}\right] = -\frac{\lambda^2}{2m\omega^2}$$

So, $$E_n = E_n^{(0)} + E_n^{(1)} + E_n^{(2)} = \left(n + \frac{1}{2}\right)\hbar\omega - \frac{\lambda^2}{2m\omega^2}$$

Energy difference between two levels is

$$(E_1 - E_0) = \left(\frac{3}{2}\hbar\omega - \frac{\lambda^2}{2m\omega^2}\right) - \left(\frac{1}{2}\hbar\omega - \frac{\lambda^2}{2m\omega^2}\right) = \hbar\omega$$

Correct answer is (d)

9. The ground state eigenfunction for the potential $V(x) = -\delta(x)$, where $\delta(x)$ is the delta function, is given by $\psi(x) = Ae^{-\alpha|x|}$, where A and $\alpha > 0$ are constants. If a perturbation $H' = bx^2$ is applied, the first order correction to the energy of the ground state will be **[CSIR June 2014]**

(a) $\frac{b}{\sqrt{2}\alpha^2}$ (b) $\frac{b}{\alpha^2}$ (c) $\frac{2b}{\alpha^2}$ (d) $\frac{b}{2\alpha^2}$

Soln. First order correction to ground state energy

$$E_0^{(1)} = \frac{\langle\psi|H'|\psi\rangle}{\langle\psi|\psi\rangle} = \int_{-\infty}^{\infty} A^2 e^{-2\alpha|x|}.bx^2 dx \Big/ \int_{-\infty}^{\infty} A^2 e^{-2\alpha|x|}dx$$

$$= 2\int_0^{\infty} e^{-2\alpha x} bx^2 dx \Big/ 2\int_0^{\infty} e^{-2\alpha x}dx = \left[b.\frac{2!}{(2\alpha)^3}\right] \Big/ \frac{1}{(2\alpha)} = \frac{b}{2\alpha^2}$$

[Using $\int_0^{\infty} e^{-ax}.x^n dx = \frac{n!}{a^{n+1}}$]

Correct answer is (d)

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10. The Hamiltonian H_0 for a three-state quantum system is given by the matrix $H_0 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix}$. When perturbed by $H' = \in \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$ where $\in \ll 1$, the resulting shift in the energy eigenvalue $E_0 = 2$ is

(a) $\in, -2\in$ (b) $-\in, 2\in$ (c) $\pm\in$ (d) $\pm 2\in$

Soln. Given: Unperturbed Hamiltonian $H_0 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix}$ and Perturbed Hamiltonian $H' = \varepsilon\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$

The unperturbed hamiltonian has unperturbed energy eigenvalues $E_0 = 1,2,2$, out of which $E_0 = 2$ is a degenarate eigenvalue having degenaracy 2. The normalized eigenvectors corresponding to these eigenvalues are respectively

$$|\psi_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, |\psi_2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, |\psi_3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

If $E_0^{(1)}$ is the energy correction due to the presence of the perturbation H' in the unperturbed eigen value $E_0 = 2$, then

$$\begin{vmatrix} H_{P_{22}} - E_0^{(1)} & H_{P_{23}} \\ H_{P_{32}} & H_{P_{33}} - E_0^{(1)} \end{vmatrix} = 0$$

where $H_{P_{22}} = \langle \psi_2 | H' | \psi_2 \rangle = \begin{pmatrix} 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = 0$

$$H_{P_{23}} = \langle \psi_2 | H' | \psi_3 \rangle = \begin{pmatrix} 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = \varepsilon$$

$$H_{P_{32}} = \langle \psi_3 | H' | \psi_2 \rangle = \begin{pmatrix} 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \varepsilon$$

$$H_{P_{33}} = \langle \psi_3 | H' | \psi_3 \rangle = \begin{pmatrix} 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = 0$$

So, $\begin{vmatrix} -E_0^{(1)} & \varepsilon \\ \varepsilon & -E_0^{(1)} \end{vmatrix} = 0 \quad \Rightarrow E_0^{(1)} = \pm\varepsilon$

Correct option is (c)

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PRACTICE SET

1. A quantum harmonic oscillator is in the energy eigenstate $|n\rangle$. A time independent perturbation $\lambda\left(a^{\dagger}a\right)^2$ acts on the particle, where λ is a constant of suitable dimensions and a and $a^{\dagger}$ are lowering and raising operators respectively. Then the first order energy shift is gien by **[GATE 2001]**

(a) λn (b) $\lambda^2 n$ (c) λn^2 (d) $(\lambda n)^2$

2. The wave function of a one-dimensional harmonic oscillator is $\psi_0 = A\exp\left(\frac{-\alpha^2 x^2}{2}\right)$ for the ground state $E_0(\alpha x/10)^4$, the first order change in the ground state energy is: [Given: $\left[(x+1)=\int_0^{\infty} t^x \exp(-t)\,dt\right]$ **[GATE 2004]**

(a) $\left(\frac{1}{2}E_0\right)10^{-4}$ (b) $(3E_0)10^{-4}$ (c) $\left(\frac{3}{4}E_0\right)10^{-4}$ (d) $(E_0)10^{-4}$

Common data for Q.3, Q.4 and Q.5

An unperturbed two-level system has energy eigenvalues E1 and E2, and eigen functions $\begin{pmatrix}1\\0\end{pmatrix}$ and $\begin{pmatrix}0\\1\end{pmatrix}$.

When perturbed, its Hamiltonian is represented by $\begin{pmatrix}E_1 & A\\ A^* & E_2\end{pmatrix}$ **[GATE 2006]**

3. The first-order correction to E_1 is:
(a) 4A (b) 2A (c) A (d) 0

4. The second-order correction to E_1 is
(a) 0 (b) A (c) $\frac{A^2}{E_2-E_1}$ (d) $\frac{A^2}{E_1-E_2}$

5. The first-order correction to the eigenfunction $\begin{pmatrix}1\\0\end{pmatrix}$ is:
(a) $\begin{pmatrix}0\\A^*/(E_1-E_2)\end{pmatrix}$ (b) $\begin{pmatrix}0\\1\end{pmatrix}$ (c) $\begin{pmatrix}A^*/(E_1-E_2)\\0\end{pmatrix}$ (d) $\begin{pmatrix}1\\1\end{pmatrix}$

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6. A particle of mass m is confined in an infinite potential well: **GATE 2010]**

$$V(x)=\begin{cases}0 & \text{if } 0<x<L,\\ \infty & \text{otherwise}\end{cases}$$

It is subjected to a perturbing potential $V_p(x)=V_0\sin\left(\frac{2\pi x}{L}\right)$ within the well. Let $E^{(1)}$ and $E^{(2)}$ be the corrections to the ground state energy in the first and second order in V_0, respectively. Which of the following are true?

(a) $E^{(1)}=0;\ E^{(2)}<0$ (b) $E^{(1)}>0;\ E^{(2)}=0$

(c) $E^{(1)}=0;\ E^{(2)}$ depends on the sign of V_0 (d) $E^{(1)}<0;\ E^{(2)}<0$

7. The normalized eigenstates of a particle in a one-dimensional potential well

$$V(x)=\begin{cases}0 & \text{if } 0<x<a\\ \infty & \text{otherwise}\end{cases}$$

are given by

$$\psi_n(x)=\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)$$

The particle is subjected to a perturbation

$$V'(x)=V_0\cos\left(\frac{\pi x}{a}\right) \quad \text{for } 0\le x\le\frac{a}{2}$$

$$=0 \qquad \text{otherwise}$$

[GATE 2011]

The shift in the ground state energy due tothe perturbation, in the first order perturbation theory,

(a) $\frac{2V_0}{3\pi}$ (b) $\frac{V_0}{3\pi}$ (c) $-\frac{V_0}{3\pi}$ (d) $-\frac{2V_0}{3\pi}$

8. Consider a system in the unperturbed state described by the Hamiltonian, $H_0=\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$. The system is subjected to a perturbation of the form $H=\begin{pmatrix}\delta & \delta\\ \delta & \delta\end{pmatrix}$ where $\delta<<1$. The energy eigenvalues of the perturbed system using the first order perturbation approximation are **[GATE 2012]**

(a) 1 and $(1+2\delta)$ (b) $(1+\delta)$ and $(1-\delta)$ (c) $(1+2\delta)$ and $(1-2\delta)$ (d) $(1+\delta)$ and $(1-2\delta)$

Common Data for Q. 9 and Q. 10:

To the given unperturbed Hamiltonian $\begin{bmatrix}5 & 2 & 0\\ 2 & 5 & 0\\ 0 & 0 & 2\end{bmatrix}$

we add a small perturbation given by $\varepsilon\begin{bmatrix}1 & 1 & 1\\ 1 & 1 & 1\\ 1 & 1 & 1\end{bmatrix}$ **[GATE 2013]**

where ε is a small quantity.

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9. The ground state eigen vector of the unperturbed Hamiltonian is

(a) $(1/\sqrt{2},1/\sqrt{2},0)$ (b) $(1/\sqrt{2},-1/\sqrt{2},0)$ (c) (0, 0, 1) (d) (1, 0, 0)

10. A pair of eigen values of the perturbed Hamiltonian, using first order perturbation theory, is

(a) $3+2\varepsilon, 7+2\varepsilon$ (b) $3+2\varepsilon, 2+\varepsilon$ (c) $3, 7+2\varepsilon$ (d) $3, 2+2\varepsilon$

11. A particle is confined in a one-dimensional potential box with the potential

$$V(x)=\begin{cases}0 & \text{if } 0<x<a\\ \infty & \text{otherwise}\end{cases}$$

If the particle is subjected to a perturbation, within the box, $W=\beta x$, where β is a small constant, the first order correction to the ground state energy is **[GATE 2014]**

(a) 0 (b) $\frac{a\beta}{4}$ (c) $\frac{a\beta}{2}$ (d) $a\beta$

12. A charged particle is in the ground state of a one-dimensional harmonic oscillator potential, generated by electrical means. If the power is suddenly switched off, so that the potential disappears, then, according to quantum mechanics, **[TIFR 2010]**

(a) the particle will shoot out of the well and move out towards infinity in one of the two possible direction as

(b) the particle will stop oscillating and as time increases it may be found farther and farther way from the centre of the well

(c) the particle will keep oscillating about the same mean position but with increasing amplitude as time increases

(d) the particle will undergo a transition to one of the higher excited states of the harmonic oscillator

13. A particle of mass 'm' and charge 'e' is in the ground state of a one-dimensional harmonic oscillator potential in the presence of a uniform external electric field E. The total potential felt by the particle is

$$V(x)=\frac{1}{2}kx^2-eEx$$ **[TIFR 2014]**

If the electric field is suddenly switched off, then the particle will

(a) Make a transition to any harmonic oscillator state with $x=-eE/k$ as origin without emitting any photon.

(b) Make a transition to any harmonic oscillator state with $x=0$ as origin and absorb a photon.

(c) Settle into the harmonic oscillator ground state with $x=0$ as origin after absorbing a photon.

(d) Oscillate back and forth with initial amplitude eE/k, emitting multiple photons as it does so.

14. A particle of mass m is contained in a one-dimensional infinite well extending from x = –L/2 to x = L/2. The particle is in its ground state given by $\psi_0(x)=\sqrt{2/L}\cos(\pi x/L)$. The walls of the box are moved suddenly to form a box extending from x = –L to x = L. What is the probability that the particle will be in the ground state after this sudden expansion? **[JEST 2013]**

(a) $(8/3\pi)^2$ (b) 0 (c) $(16/3\pi)^2$ (d) $(4/3\pi)^2$

Chapter 8

Scattering Theory

8.1 Introduction :

In scattering experiment, one observes the collission between the beam of incident particles and target material (scattering material) and their energies and angular distributions are measured. In this process, the target may remain in its original state (elastic scattering) or changes to different state (inelastic scattering).

8.2 Scattering cross-section :

Consider a beam of particles each of mass 'm' travelling along z axis with velocity v and scattered by a scattering potential V (target material) centered at the origin. The incident particles will experience a force when they are inside a sphere of radius r_0 centered at the origin, known as the range of the scattering potential. Due to the interaction of the incident particles with the scattering potential, they get scattered on all directions. After leaving the sphere, the incident particles move again along a straight line. The angle between the initial and final straight line pathgs is called scattering angle (θ).

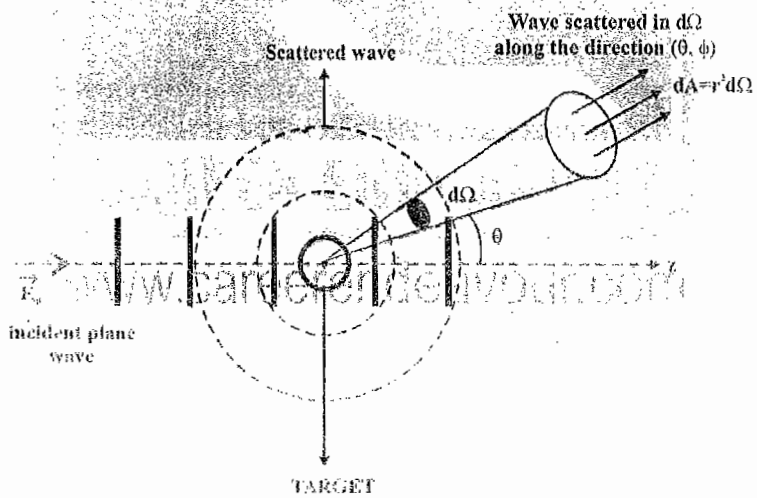

Fig.1: Schematic diagram of the scattering experiment

The total number of collisions over the duration of the experiment is proportional to the total number of incidents particles and to number of target particles per unit of area in the path of the beam. The number of particles scattered into an element of solid angle $d\Omega = \sin\theta d\theta d\phi$ is proportional to differential cross-section.

Differential scattering cross-section:

It is defined as the number of particles scattered into element of solid angle $d\Omega = \sin\theta d\theta d\phi$ in a direction (θ, ϕ) per unit time and per unit incident flux and is given by

$$\frac{d\sigma(\theta,\phi)}{d\Omega} = \frac{1}{J_{in}} \frac{dN(\theta,\phi)}{d\Omega}$$

where J_{in} is the incident flux i.e. number of incident particles per unit area per unit time and $dN(\theta,\phi)$ is the number of the particles scattered into the solid angle $d\Omega = \sin\theta d\theta d\phi$ in a direction (θ, ϕ) per unit time.

Total cross section:

It is defined as the total number of particles scattered per unit incident flux per unit time into the whole solid angle.=and given by

$$\sigma_t = \int \frac{d\sigma}{d\Omega} d\Omega = \int_0^{\pi}\int_0^{2\pi} \frac{d\sigma}{d\Omega} \sin\theta d\theta d\phi$$

For spherically symmetric potential, $\sigma(\theta,\phi)$ becomes

$$\sigma(\theta) = 2\pi \int_0^{\pi} \frac{d\sigma(\theta)}{d\Omega} \sin\theta d\theta$$

Both differential cross section and total cross section have a dimension of area and are usually measured in the units barn $\left(1 \text{ barn} = 10^{-28} m^2\right)$.

8.3 Scattering Amplitude :

At large distances from the scatterer, the effect of the scattering potential is negligible and the parallel beam of the incident particles can be represented by the plane wave $\psi_{inc}(\vec{r}) = Ae^{i\vec{k}_0 \cdot \vec{r}}$. As the incident beam is along z axis, then $\psi_{inc}(\vec{r}) = Ae^{ik_0 z}$ i.e. before the interaction with the target, the particles with incident beam are independent of each other and they move like free particles with momentum $\vec{P} = \hbar\vec{k}_0$.

When the incident wave collides with the target material, an outgoing wave is scattered out. In case of isotropic scattering, the scattered wave will be of the spherically symmetric form

$$\psi_{sca}(\vec{r}) = \frac{e^{i\vec{k}.\vec{r}}}{r}.$$

In general, the scattered wave is not spherically symmetric, its amplitude depends on the direction (θ, ϕ) along which is scattered. Therefore, the spherically diverging scattered wave can be written as,

$$\psi_{sca}(\vec{r}) = A f(\theta,\phi) \frac{e^{i\vec{k}.\vec{r}}}{r}$$

where $f(\theta,\phi)$ is known as the scattering amplitude.

For spherically symmetric potentials,

$$\psi_{sca}(\vec{r}) = A f(\theta) \frac{e^{i\vec{k}.\vec{r}}}{r}$$

where θ is the angle between $\vec{k}$ and $\vec{r}$

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The most general asymptotic solution can be wriiten as a superposition of incident plane wave and scattered wave i.e.

$$\psi(\vec{r}) = \psi_{inc}(\vec{r}) + \psi_{sca}(\vec{r}) \approx A\left[e^{ik_0 z} + f(\theta,\phi)\frac{e^{i\vec{k}.\vec{r}}}{r}\right]$$

Incident flux density $\vec{J}_{inc} = \frac{i\hbar}{2\mu}\left[\psi_{inc}\vec{\nabla}\psi^*_{inc} - \psi^*_{inc}\vec{\nabla}\psi_{inc}\right] = |A|^2\frac{\hbar k_0}{\mu}$

Scattered flux density $\vec{J}_{sca} = \frac{i\hbar}{2\mu}\left[\psi_{sca}\vec{\nabla}\psi^*_{sca} - \psi^*_{sca}\vec{\nabla}\psi_{sca}\right] = |A|^2\frac{\hbar k}{\mu r^2}|f(\theta,\phi)|^2$

where μ is the reduced mass of the system.

Number of particles that scattered per unit area per unit time = J_{sca}.

Number of particles that scattered into an element of solid angle $d\Omega$ in the direction (θ,ϕ) and passing through a surface element $dA = r^2 d\Omega$ per unit time $= dN(\theta,\phi) = J_{sca} r^2 d\Omega$

$$\Rightarrow \quad \frac{dN}{d\Omega} = J_{sca}.r^2 = |A|^2\frac{\hbar k}{\mu}|f(\theta,\phi)|^2$$

Therefore, the differential cross section $\frac{d\sigma}{d\Omega} = \frac{1}{J_{inc}}\frac{dN}{d\Omega} = \frac{k}{k_0}|f(\theta,\phi)|^2$

For elastic scattering $k = k_0 \Rightarrow \frac{d\sigma}{d\Omega} = |f(\theta,\phi)|^2$

8.4 First Born Approximation :

If the scattering potential $V(\vec{r})$ is weak enough, it will slightly distort the incident plane wave. The first born approximation consists of approximating the scattered wave as a plane wave. In this approximation, Scattering amplitude is given by

$$f(\theta,\phi) = -\frac{\mu}{2\pi\hbar^2}\int e^{i(\vec{k}_0 - \vec{k})\cdot\vec{r}}V(\vec{r})\,d\tau = -\frac{\mu}{2\pi\hbar^2}\int e^{i\vec{q}.\vec{r}}V(\vec{r})\,d\tau$$

where $\vec{q}$ is the momentum transfer and is given by

$$|\vec{q}| = |\vec{k}_0 - \vec{k}| = \sqrt{|\vec{k}_0|^2 + |\vec{k}|^2 - 2|\vec{k}||\vec{k}_0|\cos\theta} = 2k\sin\frac{\theta}{2}$$

For a spherically symmetric potential i.e. $V(\vec{r}) = V(r)$ and the corresponding scattering amplitude is

$$f(\theta) = -\frac{2\mu}{q\hbar^2}\int_0^\infty r\sin qrV(r)\,dr$$

Therefore, the differential cross section can be written as

$$\frac{d\sigma}{d\Omega} = |f(\theta,\phi)|^2 = \frac{4\mu^2}{\hbar^4 q^2}\left|\int_0^\infty r\sin qrV(r)\,dr\right|^2$$

Note: First Born approximation is valid for large incident energies and weak scattering potentials. When the average interaction energy between the incident particles and scattering potentials is much smaller than particles incident K.E., then scattered wave can be considered to be plane wave.

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Example 1: Consider the scattering of a particle having charge $Z'e$ by an atomic nucleus of charge Ze. If the potential representing the interaction is

$$V(r) = -\frac{ZZ'e^2}{r}e^{-\alpha r}$$

where α is a parameter. Calculate the scattering amplitude.

Soln. In the first Born approximation, for spherically symmetric potentials, the scattering amplitude is

$$f(\theta) = -\frac{2\mu}{q\hbar^2}\int_0^\infty r\sin qrV(r)dr = \frac{2ZZ'e^2\mu}{q\hbar^2}\int_0^\infty \sin qre^{-\alpha r}dr$$

Using the standard integral, $\int_0^\infty e^{-ax}\sin bxdx = \frac{b}{a^2+b^2}$, we get

$$f(\theta) = \frac{2\mu ZZ'e^2}{q\hbar^2}\frac{q}{q^2+\alpha^2} = \frac{2\mu ZZ'e^2}{\hbar^2\left(q^2+\alpha^2\right)}$$

where the momentum transfer $|q| = 2|k|\sin\frac{\theta}{2}$

Example 2: Find the scattering amplitude in the Born approximation for scattering by the Yukawa potential.

$$V(r) = V_0\exp\frac{-\alpha r}{r}$$

where V_0 and α are constants.

Soln. In the first Born approximation, for spherically symmetric potentials, the scattering amplitude is

$$f(\theta) = -\frac{2\mu}{q\hbar^2}\int_0^\infty V(r)r\sin qrdr = -\frac{2\mu V_0}{q\hbar^2}\int_0^\infty e^{-\alpha r}\sin qrdr$$

Using the standard integral, $\int_0^\infty e^{-ax}\sin bxdx = \frac{b}{a^2+b^2}$, we get

$$f(\theta) = -\frac{2\mu V_0}{\hbar^2\left(q^2+\alpha^2\right)} = -\frac{2\mu V_0}{\hbar^2\left(\alpha^2+4k^2\sin^2\theta/2\right)}$$

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Example 3: Using Born approximation, calculate the differential and total cross-sections for scattering of a particle of mass 'm' by the δ – function potential $V(\vec{r}) = g\delta(\vec{r})$. g – constant

Soln. In the first Born approximation, the scattering amplitude can be written as

$$f(\theta,\phi) = -\frac{m}{2\pi\hbar^2}\int e^{i\vec{q}.\vec{r}}V(\vec{r})d\tau = -\frac{mg}{2\pi\hbar^2}\int e^{i\vec{q}.\vec{r}}\delta(\vec{r})d\tau$$

Using the property of 3-D Dirac δ-function, we get

$$f(\theta) = -\frac{mg}{2\pi\hbar^2}$$

The differential scattering cross-section is

$$\sigma(\theta)=|f(\theta)|^2=\frac{m^2g^2}{4\pi^2\hbar^4}$$

Since the distribution is isotropic, the total cross-section is given by

$$\sigma=4\pi\sigma(\theta)=\frac{m^2g^2}{\pi\hbar^4}$$

Example 4: In the Born approximation, calculate the scattering amplitude for scattering from the square well potential $V(r)=-V_0$ for $0<r<r_0$ and $V(r)=0$ for $r>r_0$.

Soln. In the first Born approximation, for spherically symmetric potentials, the scattering amplitude is

$$f(\theta)=-\frac{2\mu}{q\hbar^2}\int_0^\infty V(r)r\sin qrdr=\frac{2\mu V_0}{\hbar^2q}\int_0^{r_0}r\sin qrdr$$

$$f(\theta)=\frac{2\mu V_0}{q\hbar^2}\left\{\left[\frac{r\cos qr}{-q}\right]_0^{r_0}+\frac{1}{q}\int_0^{r_0}\cos qrdr\right\}$$

$$=\frac{2\mu V_0}{\hbar^2q}\left(-\frac{r_0\cos qr_0}{q}+\frac{\sin qr_0}{q^2}\right)=\frac{2\mu V_0}{\hbar^2q^3}(\sin qr_0-qr_0\cos qr_0)$$

Example 5: A particle of mass 'm' and energy E is scattered by a spherically symmetric potential $A\delta(r-a)$, where A and a are constants. Calculate the differential scattering cross-section when the energy is very high.

Soln. At high energies, the Born approximation is more appropriate. n the first Born approximation, for spherically symmetric potentials, the scattering amplitude is

$$f(\theta)=-\frac{2m}{q\hbar^2}\int_0^\infty V(r)r\sin qrdr=-\frac{2mA}{q\hbar^2}\int_0^\infty r\sin qr.\delta(r-a)dr=-\frac{2mA}{q\hbar^2}a\sin qa$$

The differential scattering cross-section,

$$\sigma(\theta)=|f(\theta)|^2=\frac{4m^2A^2a^2\sin^2qa}{q^2\hbar^4}$$

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8.5 Partial Wave Analysis :

In this analysis, the incident plane wave is taken to be equivalent to the superposition of an infinite number of spherical waves and individual spherical waves are called partial waves. The waves with $l=0, 1, 2, \ldots\ldots$ are known as s waves, p waves, d waves and so on.

For the incident wave coming along z-axis.

$$\psi_{inc}(\vec{r})=e^{ikz}=e^{ikr\cos\theta}$$

where, $e^{ikz}=\sum_{l=0}^{\infty}(2l+1)i^l j_l(kr)P_l(\cos\theta)$. Here $j_l(kr)$ are spherical bessel functions of order l which can be related to ordinary bessel function by the relation.

$$j_l(kr)=\sqrt{\frac{\pi}{2kr}}J_{l+\frac{1}{2}}(kr)$$

In this analysis, scattering amplitude can be written as

$$f(\theta)=\frac{1}{2ik}\sum_{\ell=0}^{\infty}(2\ell+1)\left[e^{2i\delta_\ell}-1\right]P_\ell(\cos\theta)$$

$$\Rightarrow f(\theta)=\frac{1}{k}\sum_{\ell=0}^{\infty}(2\ell+1)\,e^{i\delta_\ell}\sin\delta_\ell\,P_\ell(\cos\theta)$$

where $k^2=\frac{2\mu E}{\hbar^2}$ and δ_ℓ is the phase shift of the individual partial waves due to scattering.

The corresponding differential cross-section will be

$$\frac{d\sigma}{d\theta}=\left|f(\theta)^2\right|=\frac{1}{k^2}\left|\sum_{\ell=0}^{\infty}(2\ell+1)\,e^{i\delta_\ell}\sin\delta_\ell\,P_\ell(\cos\theta)\right|^2$$

Therefore, the total cross-section will be

$$\sigma_t=\int_0^{\pi}\int_0^{2\pi}\frac{d\sigma}{d\Omega}\sin\theta\,d\theta\,d\phi=2\pi\int_0^{\pi}\left|f(\theta,\phi)\right|^2\sin\theta\,d\theta=\frac{4\pi}{k^2}\sum_{\ell=0}^{\infty}(2\ell+1)\sin^2\delta_\ell$$

Example: For S waves $(\ell=0)$,

Scattering amplitude $f(\theta)=\frac{1}{k}e^{i\delta_0}\sin\delta_0$

Differential cross section $\frac{d\sigma}{d\Omega}=\left|f(\theta)\right|^2=\frac{1}{k^2}\sin^2\delta_0$

Total cross section $\sigma=\frac{4\pi}{k^2}\sin^2\delta_0$

Note:

(i) Total cross section does not depend upon on the scattering angle θ.

(ii) At sufficiently low energies, s-wave scattering will be dominating one. As energy increases, contributions from the higher value of ℓ values become important.

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Optical Theorem

Now, for $\theta=0$

$$f(0)=\frac{1}{k}\sum_{\ell=0}^{\infty}(2\ell+1)\,e^{i\delta_l}\sin\delta_\ell=\frac{1}{k}\sum_{\ell=0}^{\infty}(2\ell+1)\left[\cos\delta_\ell\sin\delta_\ell+i\sin^2\delta_\ell\right]$$

Now, $$\sigma_t=\frac{4\pi}{k^2}\sum_{\ell=0}^{\infty}(2\ell+1)\sin^2\delta_\ell=\frac{4\pi}{k}\mathrm{Im}\left[f(0)\right]$$

This relation is known as Optical theorem.

Phase shift:

$$\sin\delta_\ell=-\frac{2\mu k}{\hbar^2}\int_0^{\infty}V(r)\,j_l^2(kr)\,r^2dr$$

For attractive potential $V(r)=-ve$ $\Rightarrow$ positive phase shift.

For repulsive potential V(r) = + ve $\Rightarrow$ negative phase shift

Scattering length:

The length upto which the effect of scattering potential can be experienced is called scattering length a is given by

$$a = \lim_{E\to 0}\left[-f(\theta)\right] = -\frac{1}{k}e^{i\delta_0}\sin\delta_0$$

For attractive potential, a = +ve which corresponds to bound state.
For repulsive potential, a = -ve which corresponds to unbound state.

Example 6: In a scattering problem, the scattering length 'a' is defind by

$$a = \lim_{E\to 0}\left[-f(\theta)\right]$$

Show that (i) the zero eneryg cross-section $\sigma_0 = 4\pi a^2$, and (ii) for weak potential $\delta_0 = -ka$

Soln. When E is very low, only s-state is involved in the scattering. Consequently, from the scattering amplitude.

$$f_0(\theta) = \frac{1}{k}e^{i\delta_0}\sin\delta_0$$

(i) In the limit $E \to 0$, $a = -\frac{1}{k}e^{i\delta_0}\sin\delta_0 \Rightarrow \sin\delta_0 = -ka e^{-i\delta_0}$

We have,

$$\sigma_0 = \frac{4\pi}{k^2}\sin^2\delta_0 = \frac{4\pi}{k^2}k^2a^2 = 4\pi a^2$$

(ii) If the potential $V(r)$ is weak, δ_0 will be the small. Then $\exp(i\delta_0) \cong 1$ and $\delta_0 \cong \delta_0$. Hence,

Scattering amplitude $f(\theta) = \frac{\delta_0}{k} \Rightarrow a = \frac{\delta_0}{k}$ or $\delta_0 = -ka$

Example 7: In a scattering experiment, the potential is spherically symmetric and the particles are scattered at such energy that only s and p waves need be considered. If the differential cross-section $\sigma(\theta)$ can be written in the form $\sigma(\theta) = a + b\cos\theta + c\cos^2\theta$, then what are the values of a, b, c in the terms of phase shifts? What is the value of total cross-section in terms of a, b, c?

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Soln. Scattering amplitude

$$f(\theta) = \frac{1}{k}\sum_{\ell=0}^{\infty}(2\ell+1)e^{i\delta_l}P_\ell(\cos\theta)\sin\delta_l = \frac{1}{k}\left[e^{i\delta_0}\sin\delta_0 + 3e^{i\delta_1}\cos\theta\sin\delta_1\right]$$

Differential cross section

$$\frac{d\sigma}{d\theta} = |f(\theta)|^2 = \frac{1}{k^2}\left[\sin^2\delta_0 + 6\sin\delta_0\sin\delta_1\cos(\delta_0-\delta_1)\cos\theta + 9\sin^2\delta_1\cos^2\theta\right]$$

Comparing with $\sigma(\theta) = a + b\cos\theta + c\cos^2\theta$, we get

$$a = \frac{\sin^2\delta_0}{k^2}, b = \frac{6}{k^2}\sin\delta_0\sin\delta_1\cos(\delta_0-\delta_1), c = \frac{9}{k^2}\sin^2\delta_1$$

Total cross-section will be $\sigma = \frac{4\pi}{k^2}\left(\sin^2\delta_0 + 3\sin^2\delta_1\right) = 4\pi a + \frac{4\pi c}{\ldots} = 4\pi\left(a + \frac{c}{\ldots}\right)$

CSIR PREVOUS YEAR QUEATION PAPERS

1. A free particle described by a plane wave and moving in the positive z-direction undergoes scattering by a potential $V(r)=\begin{cases}V_0 & \text{if } r\le R\\ 0 & \text{if } r>R\end{cases}$ if V_0 is changes to $2V_0$, keeping R fixed, then the differential scattering cross-section, in the born approximation, [CSIR June 2012]

(a) increases to four times the original value (b) increases to twice the original value
(c) decreases to half the original value (d) decreases to one fourth the original value

Soln. In the first Born approximation, the differential scattering cross section can be written as

$$\frac{d\sigma}{d\Omega}=|f(\theta,\phi)|^2=\frac{4\mu^2}{\hbar^4q^2}\left|\int_0^\infty r\sin qrV(r)dr\right|^2$$

If V_0 is changes to $2V_0$, keeping R fixed, differential scattering cross section increases to four times the original value.

Correrct option is (a)

2. In the Born approximation, the scattering amplitude $f(\theta)$ for the Yukawa potential $V(r)=\frac{\beta e^{-\mu r}}{r}$ is given by: (in the following $b=2k\sin\frac{\theta}{2}$, $E=\hbar^2k^2/2m$) [CSIR June 2013]

(a) $-\frac{2m\beta}{\hbar^2(\mu^2+b^2)^2}$ (b) $\frac{2m\beta}{\hbar^2(\mu^2+b^2)}$ (c) $-\frac{2m\beta}{\hbar^2\sqrt{\mu^2+b^2}}$ (d) $-\frac{2m\beta}{\hbar^2(\mu^2+b^2)^3}$

Soln. In the Born approximation, the scattering amplitude

$$f(\theta)=\frac{-2m}{\hbar^2k}\int_0^\infty r\sin krV(r)dr \qquad \text{where } k=2k\sin\frac{\theta}{2}=b$$

$$=\frac{-2m}{\hbar^2b}\int_0^\infty r\sin brV(r)dr=\frac{-2m}{\hbar^2b}\int_0^\infty r\left(\frac{e^{ibr}-e^{-ibr}}{2i}\right)\frac{\beta e^{-\mu r}}{r}dr$$

$$=\frac{-m\beta}{i\hbar^2b}\left[\int_0^\infty e^{ibr-\mu r}dr-\int_0^\infty e^{-ibr-\mu r}dr\right]$$

$$=\frac{-m\beta}{i\hbar^2b}\left[\int_0^\infty e^{-(-ib+\mu)r}dr-\int_0^\infty e^{-(ib+\mu)r}dr\right]$$

$$=\frac{-m\beta}{i\hbar^2b}\left[\frac{1}{\mu-ib}-\frac{1}{\mu+ib}\right]=\frac{-m\beta}{i\hbar^2b}\left[\frac{\mu+ib-\mu+ib}{\mu^2+b^2}\right]=\frac{-2m\beta}{\hbar^2(\mu^2+b^2)}$$

Correct answer is (b)

3. The scattering amplitude $f(\theta)$ for the Yukawa potential $V(r) = \beta e^{-\mu r}$, where β and μ are positive constants, is given, in the Born approximation by (in the following $b = 2k \sin\frac{\theta}{2}$, $E = \hbar^2 k^2 / 2m$)

[CSIR June 2014]

(a) $-\dfrac{4m\beta\mu}{\hbar^2\left(b^2+\mu^2\right)^2}$ (b) $-\dfrac{4m\beta\mu}{\hbar^2 b^2\left(b^2+\mu^2\right)}$ (c) $-\dfrac{4m\beta\mu}{\hbar^2\sqrt{b^2+\mu^2}}$ (d) $-\dfrac{4m\beta\mu}{\hbar^2\left(b^2+\mu^2\right)^3}$

Soln: Given : $V(r) = \beta e^{-\mu r}$ (spherically symmetric potential).

Using First Born approximation,

Scattering amplitude $f(\theta,\phi) = -\dfrac{2m}{b\hbar^2}\int_0^\infty r\sin br.V(r)\,dr$

$$\Rightarrow \quad f(\theta,\phi) = -\frac{2m}{b\hbar^2}\int_0^\infty r\sin br.\beta.e^{-\mu r}dr = -\frac{2m\beta}{b\hbar^2}\int_0^\infty e^{-\mu r}(r\sin br)\,dr$$

Using, Laplace transform of $r\sin br$ i.e.

$$L(r\sin br) = \int_0^\infty e^{-sr}(r\sin br)\,dr$$

$$\Rightarrow \quad (-1)^1\frac{d}{ds}\left[\frac{b}{s^2+b^2}\right] = \int_0^\infty e^{-sr}(r\sin br)\,dr \quad \Rightarrow \quad \frac{2sb}{\left(s^2+b^2\right)^2} = \int_0^\infty e^{-sr}(r.\sin br)\,dr$$

Therefore, $f(\theta) = -\dfrac{4m\beta\mu}{\hbar^2\left(b^2+\mu^2\right)^2}$

Correct answer is (a).

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PRACTICE SET

1. If σ is the total cross-section and $f(\theta)$, θ being the angle of scattering is the scattering amplitude for a quantum mechanical elastic scattering by a spherically symmetric potential, then which of the following is true? Note that k is the magnitude of the wave vector along the $\hat{z}$ direction.

[GATE 2002]

(a) $\sigma = |f(\theta)|^2$ (b) $\sigma = \frac{4\pi}{k}|f(\theta=0)|^2$

(c) $\sigma = \frac{4\pi}{k} \times$ imaginary part of $[f(\theta=0)]$ (d) $\sigma = \frac{4\pi}{k}|f(\theta)|^2$

Common data for Q. 2 and Q. 3

A particle is scattered by a spherically symmetric potential. In the centre of mass (CM) frame the wavefunction of the incoming particle is $\psi = Ae^{ikz}$ where k is the wavevector and A is a constant.

[GATE 2005]

2. If $f(\theta)$ is an angular function then in the asymptotic region the scattered wavefunction has the form

(a) $\frac{Af(\theta)e^{ikr}}{r}$ (b) $\frac{Af(\theta)e^{-ikr}}{r}$ (c) $\frac{Af(\theta)e^{ikr}}{r^2}$ (d) $\frac{Af(\theta)e^{-ikr}}{r^2}$

3. The differential scattering cross section $\sigma(\theta)$ in CM frame is:

(a) $\sigma(\theta) = |A|^2 \frac{|f(\theta)|^2}{r^2}$ (b) $\sigma(\theta) = |A|^2 |f(\theta)|^2$ (c) $\sigma(\theta) = |f(\theta)|^2$ (d) $\sigma(\theta) = |A||f(\theta)|$

4. For the scattering under a central force field, the asymptotic form of the total wave function after scattering is:

(a) $\psi(r) = e^{ikr} + e^{-ikr}$ (b) $\psi(r) = f(0)\frac{e^{ik.r}}{r}$

(c) $\psi(r) = e^{ik.r} + f(0)e^{ik.r}$ (d) $\psi(r) = e^{ik.r} + f(\theta)\frac{e^{ik.r}}{r}$

5. Born approximation is justified for
(a) Particle moving very slowly. (b) Very strong potential fields.
(c) Fast particles in a weak potential. (d) Hydrogen atom.

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6. A beam of quantum mechanical particles of momentum k moving along the z-direction scatters off a spherically symmetric potential

$$V(r) = \begin{cases} V_0, & \text{for } 0 \le r \le R \\ 0, & \text{for } r > R \end{cases}$$

The leading term of the wave function of the scattered particles is of the form

(a) e^{ikr} (b) e^{ikz} (c) $\frac{e^{ikr}}{r}$ (d) $\frac{e^{ikr}}{r^2}$

7. Let k be the wave number of the incident plane wave in a scattering experiment. If the scattering is purely a p-wave with the phase shift $\delta_1 = \pi/4$, then the total scattering cross-section is:

(a) $2\pi/k^2$ (b) $6\pi/k^2$ (c) 0 (d) k^2

8. For a spherically symmetric potential, $V(r) = g\delta(\vec{r})$ where $\delta(\vec{r})$ is a three dimensional δ – function and g is a constant. The scattering amplitude f(0) in the Born approximation then varies as
(a) g (b) g^2 (c) 1/g (d) $1/g^2$.

9. A beam of particles of linear momentum $\hbar k$ is scattered by a short-range potential of range a_1 where $ak << 1$. Which of the following statements is correct?
(a) All phase shifts are zero (b) There is no scattering
(c) The scattering is spherically symmetric (d) All phase shifts are equal.

10. Consider the scattering of two identical fermions. If the two particles are in a spin singlet state, the differential cross section relates to the scattering amplitude as
(a) $\frac{d\sigma}{d\Omega} = |f(\theta)|^2 + |f(\pi-\theta)|^2$ (b) $\frac{d\sigma}{d\Omega} = |f(\theta)|^2 - |f(\pi-\theta)|^2$
(c) $\frac{d\sigma}{d\Omega} = |f(\theta) - f(\pi-\theta)|^2$ (d) $\frac{d\sigma}{d\Omega} = |f(\theta) + f(\pi-\theta)|^2$

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Chapter 09

Variational and WKB method

9.1. Variational Method :

- Variation method is an approximation method to obtain the ground state energy of a quantum mechanical system.
- First we assume, some trial wave function in terms of one or more variable parameters and the value of energy is evaluated by,

$$\langle E\rangle = \langle H\rangle = \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle}$$

- Then the value of $\langle H\rangle$ is minimised w.r.t. those variable parameters. The resultant value will be the minimum value of energy.
- Energy calculated by variational method will be equal or greater than exact energy E_0 i.e. $\langle H\rangle \geq E_0$.

Example 1: Optimize the trial function $\exp(-\alpha r)$ and evaluate the ground state energy of the hydrogen atom.

Soln. Hamiltonian of the atom $H = -\frac{\hbar^2}{2\mu}\nabla^2 - \frac{ke^2}{r}$

The trial function depends only on r. Hence, ∇^2 in the spherical polar coordinates will be

$$\nabla^2 = \frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right) = \frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}$$

Now, $\langle \phi | H | \phi \rangle = -\frac{\hbar^2}{2\mu}\left[\left\langle \phi \left| \frac{d^2}{dr^2} \right| \phi \right\rangle + \left\langle \phi \left| \frac{2}{r}\frac{d}{dr} \right| \phi \right\rangle\right] - \left\langle \phi \left| \frac{ke^2}{r} \right| \phi \right\rangle$

$$= -\frac{\hbar^2}{2\mu}\left[4\pi\alpha^2\int_0^\infty r^2\exp(-2\alpha r)\,dr - 8\pi\alpha^2\int_0^\infty r\exp(-2\alpha r)\,dr\right] - 4\pi\alpha^2\int_0^\infty r\exp(-2\alpha r)\,dr$$

$$= -\frac{\hbar^2}{2\mu}\left[\frac{\pi}{\alpha} - \frac{2\pi}{\alpha}\right] - \frac{\pi ke^2}{\alpha^2}$$

and $\langle \phi | \phi \rangle = 4\pi\int_0^\infty r^2\exp(-2\alpha r)\,dr = \frac{\pi}{\alpha^3}$

Therefore, $\langle H\rangle \frac{\pi}{\alpha^3} = -\frac{\hbar^2}{2\mu}\left[\frac{\pi}{a} - \frac{2\pi}{\alpha}\right] - \frac{\pi k e^2}{\alpha^2} \Rightarrow \langle H\rangle = \frac{\hbar^2\alpha^2}{2\mu} - \alpha k e^2$

Minimizing the respect to α, we obtain

$$\frac{\partial H}{\partial \alpha} = 0 \Rightarrow \frac{\hbar^2\alpha}{\mu} - ke^2 = 0 \Rightarrow \alpha = \frac{k\mu e^2}{\hbar^2}$$

With this vlaue of α, the ground state energy of the hydrogen atom will be

$$E_{\min} = \langle H\rangle_{\min} = -\frac{\mu k^2 e^4}{2\hbar^2}$$

Example 2: Estimate the ground state energy of a one-dimensional harmonic oscillator of mass 'm' and angular frequency ω using a Gaussian trial function.

Soln. The Hamiltonian of the system $H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2$

Gaussian trial function $\phi(x) = A\exp\left(-\alpha x^2\right)$, where A and α are constants.

The normalization condition gives, $1 = |A|^2 \int_{-\infty}^{\infty} \exp\left(-2\alpha x^2\right) dx = |A|^2 \left(\frac{\pi}{2\alpha}\right)^{1/2}$

Normalized trial function $\phi(x) = \left(\frac{2\alpha}{\pi}\right)^{1/4} \exp\left(-\alpha x^2\right)$

Now, $\langle H\rangle = -\frac{\hbar^2}{2m}\left\langle \phi\left|\frac{d^2}{dx^2}\right|\phi\right\rangle + \frac{1}{2}m\omega^2\left\langle \phi\left|x^2\right|\phi\right\rangle$

$$\left\langle \phi\left|\frac{d^2}{dx^2}\right|\phi\right\rangle = -\left(\frac{2\alpha}{\pi}\right)^{1/2} 2\alpha \int_{-\infty}^{\infty} \exp\left(-2\alpha x^2\right) dx + \left(\frac{2\alpha}{\pi}\right)^{1/2} 4\alpha^2 \int_{-\infty}^{\infty} x^2 \exp\left(-2\alpha x^2\right) dx$$

$$= -\left(\frac{2\alpha}{\pi}\right)^{1/2} 2\alpha\left(\frac{\pi}{2\alpha}\right)^{1/2} + \left(\frac{2\alpha}{\pi}\right)^{1/2} 4\alpha^2 \frac{1}{4\alpha}\left(\frac{\pi}{2\alpha}\right)^{1/2} = -\alpha$$

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$$\left\langle \phi\left|x^2\right|\phi\right\rangle = \left(\frac{2\alpha}{\pi}\right)^{1/2} \int_{-\infty}^{\infty} x^2 \exp\left(-2\alpha x^2\right) dx = \frac{1}{4\alpha}$$

Therefore, $\langle H\rangle = \frac{\hbar^2\alpha}{2m} + \frac{1}{2}m\omega^2 \frac{1}{4\alpha} = \frac{\hbar^2\alpha}{2m} + \frac{m\omega^2}{8\alpha}$

Minimizing with respect to α, we get

$$0 = \frac{d\langle H\rangle}{d\alpha} = \frac{\hbar^2}{2m} - \frac{m\omega^2}{8\alpha^2} \quad or \quad \alpha = \frac{m\omega}{\hbar}$$

Therefore, $\langle H\rangle_{\min} = \frac{1}{2}\hbar\omega$

Example 3. The Schrodinger equation of a particle confined to the positive x-axis is

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2}+mgx\psi=E\psi$$

with $\psi(0)=0$, $\psi(x)\to 0$ as $x\to\infty$ and E is the energy eigenvalue. Use the trial function $x\exp(-ax)$ and obtain the best value of the parameter a.

Soln. Hamiltonian $H=\dfrac{-\hbar^2}{2m}\dfrac{d^2}{dx^2}+mgx$

Trial function, $\phi(x)=x\exp(-ax)$

$$\langle\phi|\phi\rangle=\int_0^\infty x^2\exp(-2ax)\,dx=\frac{1}{4a^3}$$

$$\left\langle\phi\left|\frac{-\hbar^2}{2m}\frac{d^2}{dx}\right|\phi\right\rangle=\frac{\hbar^2}{m}\alpha\int_0^\infty x\exp(-2\alpha x)\,dx-\frac{\hbar^2a^2}{2m}\int_0^\infty x^2\exp(-2\alpha x)\,dx$$

$$=\frac{\hbar^2}{4ma}-\frac{\hbar^2}{8ma}=\frac{\hbar^2}{8ma}$$

$$\langle\phi|mgx|\phi\rangle=mg\int_0^\infty x^3\exp(-2\alpha x)\,dx=\frac{3mg}{8a^4}$$

$$\langle H\rangle=\frac{\langle\phi|H|\phi\rangle}{\langle\phi|\phi\rangle}=\frac{\left[\hbar^2/(8ma)\right]+\left(3mg/8a^4\right)}{1/4a^3}=\frac{\hbar^2a^2}{2m}+\frac{3}{2}mga$$

Minimizing $\langle H\rangle$ with respect to a, we get

$$0=\frac{\hbar^2}{2m}2a-\frac{3}{2}mg\quad\text{or}\quad a=\left(\frac{3m^2g}{2\hbar^2}\right)^{1/3}$$

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This is the best value of the parameter 'a' such that $\langle H\rangle$ is minimum.

Example 4. Evaluate the ground state energy of a harmonic oscillator of mass 'm' and angular frequency 'ω' using the trial function.

$$\phi(x)=\begin{cases}\cos\left(\dfrac{\pi x}{2a}\right), & -a\le x\le a\\ 0, & |x|>a\end{cases}$$

Soln. $\langle H\rangle=\dfrac{\langle\phi|H|\phi\rangle}{\langle\phi|\phi\rangle}=\dfrac{\left(\dfrac{-\hbar^2}{2m}\right)\left\langle\phi\left|\dfrac{d^2}{dx^2}\right|\phi\right\rangle+\dfrac{1}{2}m\omega^2\left\langle\phi\left|x^2\right|\phi\right\rangle}{\langle\phi|\phi\rangle}$

Here, $\langle \phi | \phi \rangle = \int_{-a}^{a} \cos^2 \frac{\pi x}{2a} dx = a$

$$\left(\frac{-\hbar^2}{2m}\right)\left\langle \phi \left| \frac{d^2}{dx^2} \right| \phi \right\rangle = \frac{\hbar^2 \pi^2}{8ma^2} \int_{-a}^{a} \cos^2 \frac{\pi x}{2a} dx = \frac{\hbar^2 \pi^2}{8ma}$$

$$\left\langle \phi \left| x^2 \right| \phi \right\rangle = \int_{-a}^{a} x^2 \cos^2 \frac{\pi x}{2a} dx = \int_{-a}^{a} \frac{x^2}{2} dx + \frac{1}{2} \int_{-a}^{a} x^2 \cos \frac{\pi x}{a} dx$$

$$= \frac{a^3}{3} - \frac{2a^3}{\pi^2} = 2a^3 \left(\frac{1}{6} - \frac{1}{\pi^2}\right)$$

Therefore, $\langle H \rangle = \frac{\hbar^2 \pi^2}{8ma^2} + m\omega^2 a^2 \left(\frac{1}{6} - \frac{1}{\pi^2}\right)$

For $\langle H \rangle$ to be minimum, $\frac{\partial \langle H \rangle}{\partial a} = 0$

Taking the value of 'a' from the above condition, we get $E_{\min} = \frac{1}{2}\hbar\omega \left(\frac{\pi^2 - 6}{3}\right)^{1/2} = 0.568\hbar\omega$

Example 5. The Hamiltonian of a system is given by

$$H = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2} - a\delta(x)$$

where 'a' is a constant and $\delta(x)$ is Dirac's delta function. Estimate the ground state energy of the system using a Gaussian trial function.

Soln. The normalized Gussian trial function is given by $\phi(x) = (2b/\pi)^{1/4} \exp\left(-bx^2\right)$. Then,

$$\langle H \rangle = -\frac{\hbar^2}{2m}\left\langle \phi \left| \frac{d^2}{dx^2} \right| \phi \right\rangle - a\langle \phi | \delta(x) | \phi \rangle$$

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Here, $\left\langle \phi \left| \frac{d^2}{dx^2} \right| \phi \right\rangle = \left(\frac{2b}{\pi}\right)^{1/2} 2b \int_{-\infty}^{\infty} \exp\left(-2bx^2\right) dx + \left(\frac{2b}{\pi}\right)^{1/2} 4b^2 \int_{-\infty}^{\infty} x^2 \exp\left(-2bx^2\right) dx$

$$= -\left(\frac{2b}{\pi}\right)^{1/2} 2b \left(\frac{p}{2b}\right)^{1/2} + \left(\frac{2b}{\pi}\right)^{1/2} 4b^2 \frac{1}{4b}\left(\frac{\pi}{2b}\right)^{1/2} = -b$$

$$\langle \phi | \delta(x) | \phi \rangle = \left(\frac{2b}{\pi}\right)^{1/2} \int_{-\infty}^{\infty} \delta(x) \exp\left(-2bx^2\right) dx = \left(\frac{2b}{\pi}\right)^{1/2} \exp\left(-2bx^2\right)|_{x=0} = \left(\frac{2b}{\pi}\right)^{1/2}$$

Therefore, $\langle H \rangle = \frac{\hbar^2 b}{2m} - a\left(\frac{2b}{\pi}\right)^{1/2}$

Minimizing $\langle H \rangle$ with respect to b, we get $b = \frac{2m^2a^2}{\pi\hbar^4}$

Therefore, $\langle H \rangle_{\min} = -\frac{ma^2}{\pi\hbar^2}$

Example 6. A particle of mass 'm' is moving in a one-dimensional box defined by the potential $V = 0, 0 \le x \le a$ and $V = \infty$ otherwise. Estimate the ground state energy using the trial function

$$\psi(x) = Ax(a-x), \quad 0 \le x < a.$$

Soln. Normalization condition:

$$\langle \psi | \psi \rangle = A^2 \int_0^a x^2 (a-x)^2 = 1 \Rightarrow A^2 \left[\int_0^a a^2x^2dx - 2a\int_0^a x^3dx + \int_0^a x^4dx \right] = 1$$

$$\Rightarrow \frac{A^2a^5}{30} = 1 \quad \Rightarrow A = \sqrt{\frac{30}{a^5}}$$

The normalized trial function is $\psi(x) = \sqrt{\frac{30}{a^5}} x(a-x), \ 0 \le x \le a$

The Hamiltonian of the system is given by $H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$

Now, $\langle H \rangle = -\frac{\hbar^2}{2m}\frac{30}{a^5}\int_0^a \left(ax - x^2\right)\frac{d^2}{dx^2}\left(ax - x^2\right)dx = \frac{30\hbar^2}{ma^5}\int_0^a \left(ax - x^2\right)dx = \frac{5\hbar^2}{ma^2} = \frac{10\hbar^2}{2ma^2}$

9.2 WKB Approximation (Wentzel-Kramers-Brilouin Method)

- This is a technique for obtainibg approximate solution of the one-dimensional Schrodinger equation.
- This method is applicable or valid only for a slowing varying potentials i.e. potential that remains almost constant over a region of several de-Broglie wavelength.
- In case of classical systems, De-broglie wavelength very very small. Therefore, we can take the potential to be constant. This is why, WKB approximation is also known as semi classical approximation.

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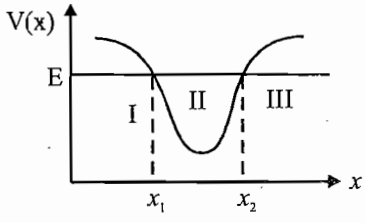
Consider a motion of a particle of mass m and energy E, in time-independent 1-D potential $V(x)$, then Schrodinger equation is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi \quad \Rightarrow \quad \frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}\left[E - V(x)\right]\psi = 0$$



II region is classically allowed region

If $E > V \Rightarrow k^2 = \frac{2m}{\hbar^2}(E-V)$ and $E < V \Rightarrow k^2 = \frac{2m}{\hbar^2}(V-E)$

Therefore, solution of the 1-D Schrodinger equation will be

$$\psi(x) = A e^{ikx} + B e^{-ikx} \qquad (E > V)$$
$$= C e^{kx} + D e^{-kx} \qquad (E < V)$$

For slowing varying potential $p(x) = \sqrt{2m(E-V(x))}$

$$\psi(x) = \frac{A}{\sqrt{p(x)}} e^{i.\frac{1}{\hbar}\int p(x)dx} + \frac{B}{\sqrt{p(x)}} e^{-i.\frac{1}{\hbar}\int p(x)dx}$$

$$= \frac{C}{\sqrt{p(x)}} e^{\frac{1}{\hbar}\int p(x)dx} + \frac{D}{\sqrt{p(x)}} e^{-\frac{1}{\hbar}\int p(x)dx}$$

$$\psi_{I,WKB} = \frac{C}{\sqrt{|p(x)|}} \exp\left[-\frac{1}{\hbar}\int_x^{x_1} |p(x)|dx\right] \qquad x < x_1$$

$$\psi_{II,WKB} = \frac{A}{\sqrt{p(x)}} \exp\left[\frac{i}{\hbar}\int p(x)dx\right] + \frac{B}{\sqrt{p(x)}} \exp\left[-\frac{i}{\hbar}\int p(x)dx\right] \qquad x_1 < x < x_2$$

$$= \frac{D}{\sqrt{|p(x)|}} \exp\left[-\frac{1}{\hbar}\int_{x_2}^{x} p(x)dx\right] \qquad x > x_2$$

In the classically allowed to region,

$$\psi_{II,WKB} = \frac{A}{\sqrt{p(x)}} \exp\left[\frac{i}{\hbar}\int p(x)dx\right] + \frac{B}{\sqrt{p(x)}} \exp\left[-\frac{i}{\hbar}\int p(x)dx\right] \qquad x_1 < x < x_2$$

$$= \frac{1}{\sqrt{p(x)}}\left[A(\cos\alpha + i\sin\alpha) + B(\cos\alpha - i\sin\alpha)\right]$$

$$= \frac{1}{\sqrt{p(x)}}\left[c_1\cos\alpha + c_2\sin\alpha\right]$$

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Taking $c_1 = A_0 \sin\beta$ and $c_2 = A_0 \cos\beta$, we get $\psi(x) = \frac{A_0}{\sqrt{p(x)}}\sin(\alpha+\beta)$

$$\Rightarrow \qquad \psi(x) = \frac{A_0}{\sqrt{p(x)}}\sin\left\{\frac{1}{\hbar}\int p(x)dx + \beta\right\}$$

where β is known as the phase factor which can take the following values:

(i) $\beta = 0$ if turning points lies on rigid walls $(V = \infty)$

(ii) $\beta = \frac{\pi}{4}$ if turning points lies on non-rigid walls $(V \neq \infty)$

But the points $x = x_i$ at which $E = V(x_i) \Rightarrow p(x_i) = 0$ are known as classical turning points because classical particle stops at x_i and returns back in motion in the opposite direction. At turning parts, wave function becomes infinte.

• Validity of WKB approximation:

$$\frac{d(\bar{\lambda})}{dx} << 1 \quad \left(\text{where } \bar{\lambda}(x) = \lambda(x)/2\pi\right) \quad \Rightarrow \frac{d}{dx}\left(\frac{\hbar}{p(x)}\right) << 1$$

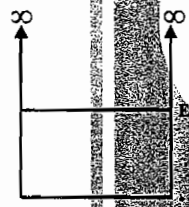
i.e. rate of change of de-Broglie wavelength is small (i.e. the DBWL must vary very slightly over the distance of the order of its size)
This system is satisfied by all classical systems.
WKB approximation is valid both for classically allowed and forbidden but not at turning points.
We will apply WKB method to find the energy levels and wave functions of the particle moving in potential well. It depends on whether or not potential well is rigid or not.

Quantaization condition of WKB aproxximation:

$$\theta_1 + \theta_2 = n\pi \quad (n = 1,2,3,.....) \quad \text{or} \quad \theta_1 + \theta_2 = (n+1)\pi \quad (n = 0,1,2,.....)$$

Example 7. Use the WKB approximation to calculate the energy of a spinless particle of mass 'm' moving in the 1-D box with walls at x = 0 and x = L

Soln.



There are 2 turning points at x = 0 and x = L.
Using the quantization condition of WKB approximation:

$$\Rightarrow \int_0^x \frac{1}{\hbar} p(x)\,dx + 0 + \int_x^L \frac{1}{\hbar} p(x)\,dx + 0 = n\pi \text{ or } (n+1)\pi$$

$$\Rightarrow \frac{1}{\hbar}\int_0^L p(x)\,dx = n\pi \text{ or } (n+1)\pi$$

$$\Rightarrow \int_0^L p(x)\,dx = n\pi\hbar \text{ or } (n+1)\pi\hbar$$

$$\Rightarrow \sqrt{2mE}.L = n\pi\hbar \text{ or } (n+1)\pi\hbar$$

$$\Rightarrow E = \frac{n^2\pi^2\hbar^2}{2mL^2} \text{ or } \frac{(n+1)^2\pi^2\hbar^2}{2mL^2}$$

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CSIR PREVIOUS YEAR QUESTIONS

1. A particle in one dimension moves under the influence of a potential $V(x) = ax^6$, where a is a real constant. large n the quantized energy level E_n depends on n as: **[CSIR June 201**

(a) $E_n \sim n^3$ (b) $E_n \sim n^{4/3}$ (c) $E_n \sim n^{6/5}$ (d) $E_n \sim n^{3/2}$

Soln. Given: A particle of mass m is moving under the following potential: $V(x) = ax^6$

At classical turning points, $E = V(x) \Rightarrow E = ax^6 \Rightarrow x = \pm\left(\frac{E}{a}\right)^{1/6} \Rightarrow x = \left(\frac{E}{a}\right)^{1/6}, -\left(\frac{E}{a}\right)^{1/6}$

Using the quantization condition of WKB approximation,

$$\int_{x_1}^{x} \sqrt{2m\left[E - V(x)\right]}\, dx + \beta_1 + \int_{x}^{x_2} \sqrt{2m\left[E - V(x)\right]}\, dx + \beta_2 = (n+1)\pi$$

According to the question, $x_1 = -\left(\frac{E}{a}\right)^{1/6}$, $x_2 = \left(\frac{E}{a}\right)^{1/6}$ and $\beta_1 = \beta_2 = \frac{\pi}{4}$ (for non-rigid walls)

Therefore, $$\int_{-(E/a)^{1/6}}^{(E/a)^{1/6}} \sqrt{2m\left[E - ax^6\right]}\, dx = \left(n + \frac{1}{2}\right)\pi$$

$$\Rightarrow \int_{-(E/a)^{1/6}}^{(E/a)^{1/6}} \underbrace{\sqrt{2m\left[E - ax^6\right]}}_{\text{dimension of } E^{1/2}} \underbrace{dx}_{\text{dimension of } E^{1/6}} = \left(n + \frac{1}{2}\right)\pi$$

So, Energy eigenvlues of the particle $E_n^{2/3} \propto \left(n + \frac{1}{2}\right) \Rightarrow E_n = \left(n + \frac{1}{2}\right)^{3/2}$

Correct answer : (d).

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2. A variational calculation is done with the normalized trial wavefunction $\psi(x) = \frac{\sqrt{15}}{4a^{5/2}}\left(a^2 - x^2\right)$ for the one dimensional potential well $V(x) = \begin{cases} 0 & \text{if } |x| \le a \\ \infty & \text{if } |x| > a \end{cases}$

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The ground state energy is estimated to be **[CSIR June 2012]**

(a) $\frac{5\hbar^3}{3ma^2}$ (b) $\frac{3\hbar^2}{2ma^2}$ (c) $\frac{3\hbar^2}{5ma^2}$ (d) $\frac{5\hbar^2}{4ma^2}$

Soln. The trial wave function $\psi(x) = \frac{\sqrt{15}}{4a^{5/2}}\left(a^2 - x^2\right)$ and $V(x) = \begin{cases} 0 & \text{if } |x| \le a \\ \infty & \text{if } |x| \ge a \end{cases}$

$$< H > = \int \psi^* H \psi\, dx = \int_{-\infty}^{+\infty} \psi^* \left(\frac{-\hbar^2}{2m}\frac{d^2}{dx^2}\right)\psi\, dx$$

$$= \int_{-\infty}^{-a} 0\left(\frac{-\hbar^2}{2m}\frac{d^2}{dx^2}\right)0\, dx + \int_{-a}^{+a} \frac{\sqrt{15}}{4a^{5/2}}\left(a^2 - x^2\right)\left(\frac{-\hbar^2}{2m}\frac{d^2}{dx^2}\right)\frac{\sqrt{15}}{4a^{5/2}}\left(a^2 - x^2\right) + \int_{+a}^{+\infty} 0\left(\frac{-\hbar^2}{2m}\frac{d^2}{dx^2}\right)0\, dx$$

$$=\frac{15}{4\times4a^5}\left(\frac{-\hbar^2}{2m}\right)\int_{-a}^{+a}\left(a^2-x^2\right)(-2)dx=\frac{15}{16\,a^5}\left(\frac{2\hbar^2}{2m}\right)\times2\int_0^a\left(a^2-x^2\right)dx$$

$$=\frac{15}{8a^5}\left(\frac{\hbar^2}{m}\right)\left(a^2x-\frac{x^3}{3}\right)_0^a=\frac{15}{8a^5}\left(\frac{\hbar^2}{m}\right)\times\frac{2}{3}a^3=\frac{5}{4}\frac{\hbar^2}{ma^2}$$

Correct answer is (d).

3. What would be the ground state energy of the Hamiltonian

$$H=-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}-\alpha\delta(x)$$

if variational principle is used to estimate it with the trial wavefunction $\psi(x)=A\,e^{-bx^2}$ with b as the variational parameter?

[Hint: $\int_{-\infty}^{\infty}x^{2n}e^{-2bx^2}dx=(2b)^{-n-\frac{1}{2}}\Gamma\left(n+\frac{1}{2}\right)$] **[CSIR Dec 2012]**

(a) $-m\alpha^2/2\hbar^2$ (b) $-2m\alpha^2/\pi\hbar^2$ (c) $-m\alpha^2/\pi\hbar^2$ (d) $m\alpha^2/\pi\hbar^2$

Soln. The Hamiltonian, $H=\frac{\hbar^2}{2m}\frac{d^2}{dx^2}-\alpha\delta(x)$

The trial wave function $\psi(x)=A\,e^{-bx^2}$ with b variational parameter.

$$\langle H\rangle=\frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}=\frac{\int_{-\infty}^{+\infty}A^*e^{-bx^2}\left(\frac{\hbar^2}{2m}\frac{d^2}{dx^2}-\alpha\delta(x)\right)Ae^{-bx^2}dx}{\int_{-\infty}^{+\infty}A^*e^{-bx^2}Ae^{-bx^2}dx}$$

$$=\frac{|A|^2\left[\int_{-\infty}^{+\infty}e^{-bx^2}\left(\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right)e^{-bx^2}dx-\alpha\int_{-\infty}^{+\infty}e^{-2bx^2}\delta(x)dx\right]}{|A|^2\int_{-\infty}^{+\infty}e^{-2bx^2}dx}$$

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$$=\frac{\frac{-\hbar^2}{2m}\int_{-\infty}^{+\infty}e^{-bx^2}\left(4b^2x^2-2b\right)e^{-bx^2}dx-\alpha}{\int_{-\infty}^{+\infty}e^{-2bx^2}dx}\qquad\left[\text{by using }\int_{-\infty}^{+\infty}f(x)\delta(x-a)dx=f(a)\right]$$

$$\langle\hat{H}\rangle=\frac{-\frac{\hbar^2}{2m}4b^2\int_{-\infty}^{+\infty}e^{-2bx^2}x^2dx+\frac{\hbar^2}{2m}2b\int_{-\infty}^{+\infty}e^{-2bx^2}dx-\alpha}{\int_{-\infty}^{+\infty}e^{-2bx^2}dx}=\frac{\frac{-4b^2\hbar^2}{2m}\int_0^{\infty}e^{-2bx^2}x^2dx+\frac{2b\hbar^2}{2m}\int_0^{\infty}e^{-2bx^2dx}-\frac{\alpha}{2}}{\int_0^{\infty}e^{-2bx^2}dx}$$

$$= \frac{\frac{-4b^2\hbar^2}{2m}\times\frac{1}{2}\frac{\sqrt{\pi/2}}{(2b)^{3/2}} + \frac{2b\hbar^2}{2m}\times\frac{\sqrt{\pi}}{2(2b)^{1/2}} - \frac{\alpha}{2}}{\frac{\sqrt{\pi}}{2(2b)^{1/2}}} = -\frac{\hbar^2 b}{2m} + \frac{2b\hbar^2}{2m} - \frac{\alpha}{\sqrt{\pi}}(2b)^{1/2} = \frac{b\hbar^2}{2m} - \frac{\alpha(2b)^{1/2}}{\sqrt{\pi}}$$

$$\frac{\partial\langle H\rangle}{\partial b} = 0 \quad \Rightarrow \frac{\hbar^2}{2m} - \frac{\alpha\times 2^{1/2}}{\sqrt{\pi}}\frac{1}{2b^{1/2}} = 0 \quad \Rightarrow \quad \frac{\alpha}{\sqrt{2\pi b}} = \frac{\hbar^2}{2m}$$

$$\Rightarrow \frac{\alpha^2}{2\pi b} = \frac{\hbar^4}{4m^2} \quad \Rightarrow \quad b = \frac{2\alpha^2 m^2}{\pi\hbar^4}$$

The ground state energy, $E = \frac{\hbar^2}{2m}\left(\frac{2\alpha^2m^2}{\pi\hbar^4}\right) - \frac{\alpha\times 2^{1/2}}{\sqrt{\pi}}\left(\frac{2\alpha^2m^2}{\pi\hbar^4}\right)^{1/2}$

$$= \frac{\alpha^2 m}{\pi\hbar^2} - \frac{2\alpha^2 m}{\pi\hbar^2} = -\frac{\alpha^2 m}{\pi\hbar^2}$$

Correct option is (c)

4. The bound on the ground state energy of the Hamiltonian with an attractive delta-function potential, namely

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - \alpha\delta(x)$$

using the variational principle with the trial wavefunction $\psi(x) = A\exp(-bx^2)$ is

[CSIR June 2013]

(a) $-m\alpha^2/4\pi\hbar^2$ (b) $-m\alpha^2/2\pi\hbar^2$ (c) $-m\alpha^2/\pi\hbar^2$ (d) $-m\alpha^2/\sqrt{5}\pi\hbar^2$

Soln. The Hamiltonian, $H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - \alpha\delta(x)$

The trial wave function $\psi(x) = Ae^{-bx^2}$ with b variational parameter.

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$$\langle H\rangle = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{\int_{-\infty}^{+\infty} Ae^{-bx^2}\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right)Ae^{-bx^2}dx - \alpha\int_{-\infty}^{+\infty} Ae^{-bx^2}\delta(x)Ae^{-bx^2}dx}{\int_{-\infty}^{+\infty} A^*e^{-bx^2}\,Ae^{-bx^2}dx}$$

$$= \frac{|A|^2\int_{-\infty}^{+\infty} e^{-bx^2}\left(\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right)e^{-bx^2}dx - \alpha\int_{-\infty}^{+\infty} e^{-2bx^2}\delta(x)dx\right)}{|A|^2\int_{-\infty}^{+\infty} e^{-2bx^2}dx}$$

$$= \frac{\frac{-\hbar^2}{2m}\int_{-\infty}^{+\infty} e^{-bx^2}\left(4b^2x^2 - 2b\right)e^{-bx^2}dx - \alpha}{\int_{-\infty}^{+\infty} e^{-2bx^2}dx} \qquad \left[\text{by using } \int_{-\infty}^{+\infty} f(x)\delta(x-a)dx = f(a)\right]$$

$$\langle \hat{H} \rangle = \frac{-\frac{\hbar^2}{2m}4b^2\int_{-\infty}^{+\infty} e^{-2bx^2}x^2dx + \frac{\hbar^2}{2m}2b\int_{-\infty}^{+\infty} e^{-2bx^2}dx - \alpha}{\int_{-\infty}^{+\infty} e^{-2bx^2}dx} = \frac{\frac{-4b^2\hbar^2}{2m}\int_0^{\infty} e^{-2bx^2}x^2dx + \frac{2b\hbar^2}{2m}\int_0^{\infty} e^{-2bx^2dx} - \frac{\alpha}{2}}{\int_0^{\infty} e^{-2bx^2}dx}$$

$$= \frac{\frac{-4b^2\hbar^2}{2m}\times\frac{1}{2}\frac{\sqrt{\pi/2}}{(2b)^{3/2}} + \frac{2b\hbar^2}{2m}\times\frac{\sqrt{\pi}}{2(2b)^{1/2}} - \frac{\alpha}{2}}{\frac{\sqrt{\pi}}{2(2b)^{1/2}}} = -\frac{\hbar^2 b}{2m} + \frac{2b\hbar^2}{2m} - \frac{\alpha}{\sqrt{\pi}}(2b)^{1/2} = \frac{b\hbar^2}{2m} - \frac{\alpha(2b)^{1/2}}{\sqrt{\pi}}$$

$$\frac{\partial\langle H\rangle}{\partial b} = 0 \quad \Rightarrow \frac{\hbar^2}{2m} - \frac{\alpha\times 2^{1/2}}{\sqrt{\pi}}\frac{1}{2b^{1/2}} = 0 \quad \Rightarrow \quad \frac{\alpha}{\sqrt{2\pi b}} = \frac{\hbar^2}{2m}$$

$$\Rightarrow \frac{\alpha^2}{2\pi b} = \frac{\hbar^4}{4m^2} \quad \Rightarrow \quad b = \frac{2\alpha^2m^2}{\pi\hbar^4}$$

The ground state energy, $E = \frac{\hbar^2}{2m}\left(\frac{2\alpha^2m^2}{\pi\hbar^4}\right) - \frac{\alpha\times 2^{1/2}}{\sqrt{\pi}}\left(\frac{2\alpha^2m^2}{\pi\hbar^4}\right)^{1/2}$

$$= \frac{\alpha^2m}{\pi\hbar^2} - \frac{2\alpha^2m}{\pi\hbar^2} = -\frac{\alpha^2m}{\pi\hbar^2}$$

Correct answer is (c)

5. Consider a particle of mass m in the potential $V(x) = a|x|, a > 0$. The energy eigen-values $E_n (n = 0,1,2,...)$, in the WKB approximation, are **[CSIR Dec 2014]**

(a) $\left[\frac{3a\hbar\pi}{4\sqrt{2m}}\left(n+\frac{1}{2}\right)\right]^{1/3}$ (b) $\left[\frac{3a\hbar\pi}{4\sqrt{2m}}\left(n+\frac{1}{2}\right)\right]^{2/3}$ (c) $\frac{3a\hbar\pi}{4\sqrt{2m}}\left(n+\frac{1}{2}\right)$ (d) $\left[\frac{3a\hbar\pi}{4\sqrt{2m}}\left(n+\frac{1}{2}\right)\right]^{4/3}$

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Soln. Given: A particle of mass m is moving under the following potential $V(x) = a|x|$

At classical turning points, $E = V(x) \Rightarrow E = a|x| \Rightarrow |x| = \frac{E}{a} \Rightarrow x = \frac{E}{a}, -\frac{E}{a}$

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Using the quantization condition of WKB approximation,

$$\int_{x_1}^{x}\sqrt{2m[E-V(x)]}\,dx + \beta_1 + \int_{x}^{x_2}\sqrt{2m[E-V(x)]}\,dx + \beta_2 = (n+1)\pi$$

According to the question, $x_1 = -\frac{E}{a}$, $x_2 = \frac{E}{a}$ and $\beta_1 = \beta_2 = \frac{\pi}{4}$ (for non-rigid walls)

Therefore, $\int_{-E/a}^{E/a}\sqrt{2m[E-a|x|]}\,dx = \left(n+\frac{1}{2}\right)\pi$

$$\Rightarrow \int_{-E/a}^{E/a}\underbrace{\sqrt{2m[E-a|x|]}}_{\text{dimension of } E^{1/2}}\underbrace{dx}_{\text{dimension of } E} = \left(n+\frac{1}{2}\right)\pi$$

So, Energy eigenvlues of the particle $E_n^{3/2} \infty \left(n+\frac{1}{2}\right) \Rightarrow E_n = \left(n+\frac{1}{2}\right)^{2/3}$

Correct Option is (2)

6. The ground state energy of the attractive delta function potential $V(x) = -b\delta(x)$, where $b > 0$, calculatec with the variational trial function $\psi(x) = \begin{cases} A\cos\frac{\pi x}{2a}, & \text{for} -a < x < a, \\ 0, & \text{otherwise,} \end{cases}$ is **[CSIR Dec 2014]**

(a) $-\frac{mb^2}{\pi^2\hbar^2}$ (b) $-\frac{2mb^2}{\pi^2\hbar^2}$ (c) $-\frac{mb^2}{2\pi^2\hbar^2}$ (d) $-\frac{mb^2}{4\pi^2\hbar^2}$

Soln. Given: Potential $V(x) = -b\,\delta(x)$ and variational trial function

$$\psi(x) = \begin{cases} A\cos\frac{\pi x}{2a} & \text{for} -a < x < a \\ 0 & \text{otherwise} \end{cases}$$

Thus, $\langle E \rangle = \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} = \frac{\left\langle \psi \left| -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} \right| \psi \right\rangle - \langle \psi | b\,\delta(x) | \psi \rangle}{\langle \psi | \psi \rangle}$

$$= \frac{-\frac{\hbar^2}{2m}A^2\left(-\frac{\pi^2}{4a^2}\right)\int_{-a}^{a}\cos^2\frac{\pi x}{2a}dx - A^2 b\int_{-a}^{a}\cos^2\frac{\pi x}{2a}\delta(x)dx}{A^2\int_{-a}^{a}\cos^2\frac{\pi x}{2a}dx}$$

$$= \frac{\frac{\pi^2\hbar^2}{8ma^2} - \frac{b}{a}}{1}$$

Now, minimizing $\langle E \rangle$ w.r.t a i.e. putting $\frac{\partial \langle E \rangle}{\partial a} = 0$, we get

$$\Rightarrow \frac{\pi^2\hbar^2}{8m}\left(-\frac{2}{a^3}\right) + \frac{b}{a^2} = 0 \Rightarrow a = \frac{\pi^2\hbar^2}{4mb}$$

Therefore, $\langle E \rangle_{\min} = \frac{\pi^2\hbar^2}{8m\left(\frac{\pi^2\hbar^2}{4mb}\right)^2} - \frac{b}{\left(\frac{\pi^2\hbar^2}{4mb}\right)} = -\frac{2mb^2}{\pi^2\hbar^2}$

Correct Option is (b)

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